

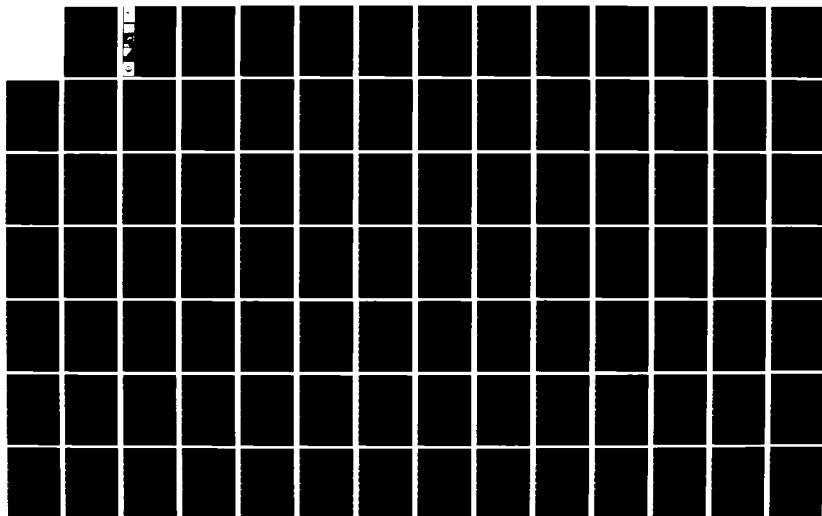
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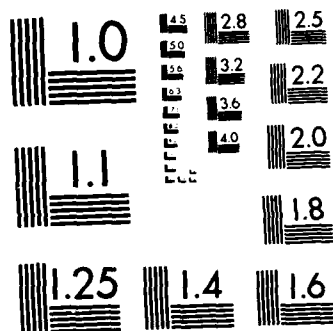
THE DEVELOPMENT OF A NUMERICAL SOLUTION TO THE  
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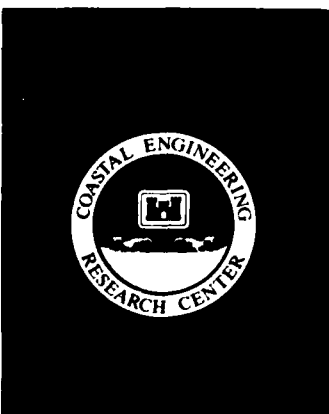




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# THE DEVELOPMENT OF A NUMERICAL SOLUTION TO THE TRANSPORT EQUATION

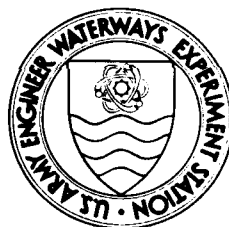
Report 1

METHODOLOGY

by

R. A. Schmalz, Jr.

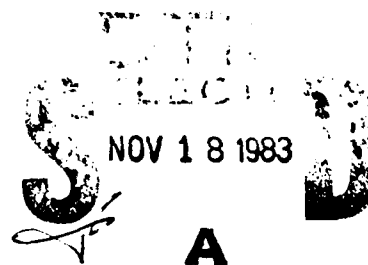
Coastal Engineering Research Center  
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September 1983

Report 1 of a Series

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Prepared for U. S. Army Engineer District, Mobile  
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20. ABSTRACT (Continued).

> and flux-corrected transport algorithms were selected for numerical implementation (Report 2) and testing (Report 3). The algorithm developed is to be included within the U. S. Army Engineer Waterways Experiment Station Implicit Flooding Model (WIFM). The model will be used to predict changes in salinity distributions due to alternative dredge disposal practices in Mississippi Sound and adjacent areas.

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## PREFACE

The methodology for the development of a numerical solution to the transport equation is reported herein. A numerical solution procedure will be developed in Report 2 of this series. Numerical test results are presented in Report 3. The solution procedure will be incorporated in a numerical model to be used for evaluating effects of proposed dredged material disposal practices in Mississippi Sound and adjacent areas.

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Literature review and methodology development were conducted by the U. S. Army Engineer Waterways Experiment Station (WES) in the Hydraulics Laboratory (HL) under the general supervision of Messrs. H. B. Simmons and F. H. Herrmann, Jr., Chief and Assistant Chief, respectively, HL, and in CERC under the general supervision of Drs. R. W. Whalin and L. E. Link, Chief and Assistant Chief, respectively, CERC, and Mr. C. E. Chatham, Chief, Wave Dynamics Division (WDD). This report was prepared by Dr. R. A. Schmalz, Jr., WDD.

Commanders and Directors of WES during data acquisition and analysis and the preparation and publication of this report were COL Nelson P. Conover, CE, and COL Tilford C. Creel, CE. Technical Director was Mr. F. R. Brown.

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# DEVELOPMENT OF A NUMERICAL SOLUTION TO THE TRANSPORT EQUATION

## Report 1: METHODOLOGY

### PART I: INTRODUCTION

This report constitutes the first report in a three-report series and develops the methodology for obtaining a numerical solution to the transport equation. The algorithm developed is to be included within the Waterways Experiment Station Implicit Flooding Model (WIFM) [1]. The development of both the vertically integrated hydrodynamic and transport equations is presented in PART II in order to point out the assumptions made in a two-dimensional approach. A literature review of current research in finite difference approximation techniques to the transport equation has been conducted in order to determine the most effective approach for simulating salinity levels in Mississippi Sound. Results are detailed in PART III. The numerical method selection and proposed form of development is the subject of PART IV.

It is instructive here to note the component tasks in the development of a mathematical model. Initially, one must decide what form of the equations is to be approximated. Certain simplifications and assumptions must be made to obtain the system of equations. Secondly, one must select a suitable numerical approximation to the equations. Next the numerical approximations must be computationally implemented. The efficacy of the approximation must then be tested by comparing simulated results against known solutions under simplified boundary and flow

conditions. Finally, empirical coefficients (friction and dispersion) must be adjusted during simulation of measured prototype conditions and subsequently verified. This report presents the results for the first two steps in this process. Subsequent steps will be presented in separate reports.

## PART II: MODEL EQUATION DEVELOPMENT

The hydrodynamic and transport equations are developed in two dimensional vertically integrated form. The time averaging concepts necessary in describing the turbulence are introduced as necessary in the derivations but are not treated in detail. An equation of state is developed which effectively couples the hydrodynamics and transport equations. Finally, the complete equation sets are presented for the coupled and uncoupled cases.

### 1. Hydrodynamic Equations

The general equations of the classical hydrodynamics for incompressible flow are given following Lai's development as follows [2].

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1.1)$$

$$\rho \frac{Du}{Dt} = \rho F_x - \frac{\partial p}{\partial x} + \mu \Delta^2 u \quad (1.2)$$

$$\rho \frac{Dv}{Dt} = \rho F_y - \frac{\partial p}{\partial y} + \mu \Delta^2 v \quad (1.3)$$

$$\rho \frac{Dw}{Dt} = \rho F_z - \frac{\partial p}{\partial z} + \mu \Delta^2 w \quad (1.4)$$

with

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z}$$

$$\Delta^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

where

$x, y, z \equiv$  Cartesian coordinates

$u, v, w \equiv$  Velocity components in the  $x$ ,  $y$ , and  $z$  directions,  
respectively

$F_x, F_y, F_z \equiv$  Body forces in the  $x$ ,  $y$ , and  $z$  directions, respectively

$\rho \equiv$  Fluid density

$\mu \equiv$  Fluid viscosity

$p \equiv$  Pressure

$t \equiv$  Time

The following assumptions are made:

1. The water is not deep compared with the length of the wave and the shallow water theory applies.
2. The vertical velocity of flow is small.
3. The vertical acceleration of the fluid particle is very small compared with the acceleration of gravity,  $g$ , and, hence, can be neglected.
4. The pressure is hydrostatic (from the above assumption).
5. The frictional resistance coefficient for unsteady flow is the same as that for steady flow, thus can be approximated from the Chézy or Manning equation.
6. Only shear stresses due to horizontal velocity components are significant.
7. The bottom of the embayment is rigid or relatively stable and fixed with respect to time.
8. The water is nonhomogenous but incompressible. The density induced flow appears only in the pressure gradient terms.

### 1.1 Continuity Equation

If we consider (1.1) and integrate over the vertical from the

bottom  $z_b(x,y)$  to the surface  $\eta(x,y,t)$  we obtain

$$\int_{z_b}^{\eta} \frac{\partial u}{\partial x} dz + \int_{z_b}^{\eta} \frac{\partial u}{\partial y} dz + w(\eta) - w(z_b) = 0 \quad (1.1.1)$$

From Leibniz rule we may write

$$\frac{\partial}{\partial x} \int_{z_b}^{\eta} u dz = u(\eta) \frac{\partial \eta}{\partial x} - u(z_b) \frac{\partial z_b}{\partial x} + \int_{z_b}^{\eta} \frac{\partial u}{\partial x} dz \quad (1.1.2)$$

$$\frac{\partial}{\partial y} \int_{z_b}^{\eta} v dz = v(\eta) \frac{\partial \eta}{\partial y} - v(z_b) \frac{\partial z_b}{\partial y} + \int_{z_b}^{\eta} \frac{\partial v}{\partial y} dz \quad (1.1.3)$$

Employ the kinematic boundary condition; namely, for  $F(x,y,z,t) = 0$  as a boundary surface assume any particle on the surface remains on it implies

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + u \frac{\partial F}{\partial x} + v \frac{\partial F}{\partial y} + w \frac{\partial F}{\partial z} = 0$$

Consider  $z = \eta(x,y,t)$  at the free surface, then

$F = z - \eta(x,y,t) = 0$  . Hence

$$\frac{DF}{Dt} = 0 \Rightarrow \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + v \frac{\partial \eta}{\partial y} = w \quad (1.1.4)$$

At the bottom  $z = z_b(x,y)$  .

Hence

$$DF/Dt = 0 \Rightarrow u \frac{\partial z_b}{\partial x} + v \frac{\partial z_b}{\partial y} = w \quad (1.1.5)$$

Returning to (1.1.1)

$$\begin{aligned} \frac{\partial}{\partial x} \int_{z_b}^{\eta} u \, dz + \underline{\underline{u(z_b) \frac{\partial z_b}{\partial x}}} - \underline{\underline{u(\eta) \frac{\partial \eta}{\partial x}}} \frac{\partial}{\partial y} \int_{z_b}^{\eta} v \, dz + \underline{\underline{v(z_b) \frac{\partial z_b}{\partial y}}} \\ - v(\eta) \frac{\partial \eta}{\partial y} + \underline{\underline{w(\eta)}} - \underline{\underline{w(z_b)}} = 0 \end{aligned} \quad (1.1.6)$$

The sum of the  $\underline{\underline{\hspace{1cm}}}$  terms is zero from the bottom boundary condition.

The sum of the  $\underline{\hspace{1cm}}$  terms is equal to  $\partial \eta / \partial t$  from the free surface boundary conditions. Thus we obtain:

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} \int_{z_b}^{\eta} u \, dz + \frac{\partial}{\partial y} \int_{z_b}^{\eta} v \, dz = 0 \quad (1.1.7)$$

Denoting

$$\bar{u} = \frac{1}{\eta - z_b} \int_{z_b}^{\eta} u \, dz \quad \text{and} \quad \bar{v} = \frac{1}{\eta - z_b} \int_{z_b}^{\eta} v \, dz$$

one obtains

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} [(\eta - z_b) \bar{u}] + \frac{\partial}{\partial y} [(\eta - z_b) \bar{v}] = 0 \quad (1.1.8)$$

Letting  $h = \eta - z_b$  and dropping the bar notation with the understanding henceforth we are considering vertically averaged quantities

one obtains

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} (hu) + \frac{\partial}{\partial y} (hv) = 0 \quad (1.1.9)$$

## 1.2 Equations of Motion

Consider the  $z$  motion equation in which  $Dw/Dt = 0$ ,  $\mu\Delta^2 w = 0$  from assumptions 2, 3 and 6, respectively. Thus we obtain

$$\rho F_z - \frac{\partial p}{\partial z} = 0 \quad (1.2.1)$$

$F_z$  is replaced by  $-g$  due to the following assumptions

1. The vertical component of the Coriolis force is negligible with respect to  $g$ .
2. The vertical tide generating force component is negligible with respect to  $g$ .

If we integrate the above relation from an arbitrary level  $z$  to the water surface obtain

$$p(z) = p(\eta) + \int_z^\eta \rho g \, dr \quad (1.2.2)$$

To depth average we consider the following relations to hold, in which the bar quantities are depth averages and the prime quantities the local fluctuation from these averages.

$$\rho(z) = \bar{\rho} + \rho'(z) \quad (1.2.3)$$

$$p(z) = \bar{p} + p'(z) \quad (1.2.4)$$

$$\int_{z_b}^\eta \rho' \, dz = \int_{z_b}^\eta p' \, dz = 0 \quad (1.2.5)$$

Taking the partial derivative of (1.2.2) with respect to  $x$  obtain:



$$\frac{\partial p}{\partial x} = \frac{\partial p(\eta)}{\partial x} + \frac{\partial}{\partial x} \left[ \int_z^\eta \rho g \, dr \right] \quad (1.2.6)$$

Integrating (1.2.6) over the vertical we write:

$$\underbrace{\int_{z_b}^\eta \frac{\partial(\bar{p} + p')}{\partial x} \, dz}_{\textcircled{1}} = \underbrace{\int_{z_b}^\eta \frac{\partial p(\eta)}{\partial x} \, dz}_{\textcircled{2}} + \underbrace{\int_{z_b}^\eta \left[ \frac{\partial}{\partial x} \int_z^\eta \rho g \, dr \right] \, dz}_{\textcircled{3}} \quad (1.2.7)$$

Let us consider terms  $\textcircled{1} - \textcircled{3}$ , separately, in turn. Evaluating  $\textcircled{1}$  invoke Leibniz rule

$$\begin{aligned} \int_{z_b}^\eta \frac{\partial}{\partial x} (\bar{p} + p') \, dz &= \frac{\partial}{\partial x} \int_{z_b}^\eta (\bar{p} + p') \, dz \\ &\quad + (\bar{p} + p') \Big|_{z_b} \frac{\partial z_b}{\partial x} - (\bar{p} + p') \Big|_\eta \frac{\partial \eta}{\partial x} \end{aligned} \quad (1.2.8)$$

Note further from (1.2.5),

$$\begin{aligned} \frac{\partial}{\partial x} \int_{z_b}^\eta (\bar{p} + p') \, dz &= \frac{\partial}{\partial x} [\bar{p}(\eta - z_b)] \\ &= (\eta - z_b) \frac{\partial \bar{p}}{\partial x} + \bar{p} \left( \frac{\partial \eta}{\partial x} - \frac{\partial z_b}{\partial x} \right) \end{aligned} \quad (1.2.9)$$

Thus we finally obtain for  $\textcircled{1}$  the following expression:

$$\int_{z_b}^\eta \frac{\partial}{\partial x} (\bar{p} + p') \, dz = (\eta - z_b) \frac{\partial \bar{p}}{\partial x} + \bar{p} \Big|_{z_b} \frac{\partial z_b}{\partial x} - \bar{p}' \Big|_\eta \frac{\partial \eta}{\partial x} \quad (1.2.10)$$

If we let  $h = \eta - z_b$  and assume  $p' \Big|_{z_b} \partial z_b / \partial x$ ,  $p' \Big|_{\eta} \partial \eta / \partial x = 0$ , then we obtain

$$\int_{z_b}^{\eta} \frac{\partial}{\partial x} (\bar{p} + p') dz = h \frac{\partial \bar{p}}{\partial x} \quad (1.2.11)$$

Evaluating ② note  $\partial p(\eta) / \partial x$  is not a function of depth; thus we obtain

$$\int_z^{\eta} \frac{\partial p(\eta)}{\partial x} dz = \frac{\partial p(\eta)}{\partial x} (\eta - z_b) = h \frac{\partial p_a}{\partial x} \quad (1.2.12)$$

where

$$p_a = p(\eta)$$

Next consider the iterated integral expression for ③ as follows:

$$\begin{aligned} \frac{\partial}{\partial x} \int_z^{\eta} \rho g dz &= g \frac{\partial}{\partial x} [\bar{\rho}(\eta - z)] \\ &= g \left[ \frac{\partial \bar{\rho}}{\partial x} (\eta - z) + \bar{\rho} \frac{\partial (\eta - z)}{\partial x} \right] \end{aligned} \quad (1.2.13)$$

Note

$$\int_{z_b}^{\eta} g \frac{\partial \bar{\rho}}{\partial x} (\eta - z) dz = g \frac{\partial \bar{\rho}}{\partial x} \int_{\eta - z_b}^0 -s ds = g \frac{\partial \bar{\rho}}{\partial x} \frac{h^2}{2} \quad (1.2.14)$$

if

$$s = \eta - z$$

$$ds = -dz$$

Observe from Leibniz rule

$$g\bar{\rho} \int_{z_b}^{\eta} \frac{\partial(\eta - z)}{\partial x} dz = g\bar{\rho} \left[ \frac{\partial}{\partial x} \int_{z_b}^{\eta} (\eta - z) dz + (\eta - z_b) \frac{\partial z_b}{\partial x} - \cancel{(\eta - \eta)} \frac{\partial \eta}{\partial x} \right] \quad (1.2.15)$$

Letting  $h = \eta - z_b$  obtain:

$$\begin{aligned} g\bar{\rho} \int_{z_b}^{\eta} \frac{\partial(\eta - z)}{\partial x} dz &= g\bar{\rho} \frac{\partial}{\partial x} \left( \frac{h^2}{2} \right) + h \frac{\partial z_b}{\partial x} \\ &= g\bar{\rho} h \left[ \frac{\partial h}{\partial x} + \frac{\partial z_b}{\partial x} \right] = g\bar{\rho} h \frac{\partial \eta}{\partial x} \end{aligned} \quad (1.2.16)$$

and the evaluation ③ is complete. Assembling all our results we obtain finally

$$h \frac{\partial \bar{p}}{\partial x} = h \frac{\partial p_a}{\partial x} + \bar{\rho} g h \frac{\partial \eta}{\partial x} + g \frac{h^2}{2} \frac{\partial \bar{\rho}}{\partial x} \quad (1.2.17)$$

Analagously, the expression for the  $y$  gradient is given by

$$h \frac{\partial \bar{p}}{\partial y} = h \frac{\partial p_a}{\partial y} + \bar{\rho} g h \frac{\partial \eta}{\partial y} + g \frac{h^2}{2} \frac{\partial \bar{\rho}}{\partial y} \quad (1.2.18)$$

Thus we have employed the  $z$  motion equation to evaluate the horizontal pressure gradients in the  $x$  and  $y$  motion equations. The expressions obtained above for these gradients include the atmospheric pressure anomaly, the water surface elevation gradient, and the density gradient created by horizontal variations in salinity and temperature.

Let us next consider the material derivative (left hand side) of

(1.2) the x motion equation. Expanding the material derivative and adding (1.1) we obtain

$$\begin{aligned} & \rho \left[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} + u \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \\ &= \rho \left[ \frac{\partial u}{\partial t} + \frac{\partial(u^2)}{\partial x} + \frac{\partial(uv)}{\partial y} + \frac{\partial(uw)}{\partial z} \right] \\ &= \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} \end{aligned} \quad (1.2.19)$$

Integrating the last result over the vertical (which also holds for compressible flow)

$$\begin{aligned} & \int_{z_b}^{\eta} \frac{\partial(\rho u)}{\partial t} dz + \int_{z_b}^{\eta} \frac{\partial(\rho u^2)}{\partial x} dz \\ &+ \int_{z_b}^{\eta} \frac{\partial(\rho uv)}{\partial y} dz + \int_{z_b}^{\eta} \frac{\partial(\rho uw)}{\partial z} dz \end{aligned} \quad (1.2.20)$$

Again employing Leibniz rule

$$\begin{aligned} \frac{\partial}{\partial t} \int_{z_b}^{\eta} (\rho u) dz &= \int_{z_b}^{\eta} \frac{\partial}{\partial t} (\rho u) dz \\ &+ \rho u \Big|_{\eta} \frac{\partial \eta}{\partial t} - (\rho u) \Big|_{z_b} \frac{\partial z_b}{\partial t} \end{aligned} \quad (1.2.21)$$

$$\frac{\partial}{\partial x} \int_{z_b}^{\eta} (\rho u u) dz = \int_{z_b}^{\eta} \frac{\partial(\rho u u)}{\partial x} dz + \rho u u \Big|_{\eta} \frac{\partial \eta}{\partial x} - \rho u u \Big|_{z_b} \frac{\partial z_b}{\partial x} \quad (1.2.22)$$

$$\frac{\partial}{\partial y} \int_{z_b}^{\eta} (\rho u v) dz = \int_{z_b}^{\eta} (\rho u v) dz + \rho u v \Big|_{\eta} \frac{\partial \eta}{\partial y} - \rho u v \Big|_{z_b} \frac{\partial z_b}{\partial y} \quad (1.2.23)$$

$$\int_{z_b}^{\eta} \frac{\partial}{\partial z} (\rho u w) dz = \rho u w \Big|_{\eta} - \rho u w \Big|_{z_b} \quad (1.2.24)$$

Notice in the above  $\partial z_b / \partial t = 0$ , since the bottom is assumed rigid. Denoting terms in (1.1.4) by ①, and those in (1.1.5) by ②, we obtain the following

$$\begin{aligned} \frac{\partial}{\partial t} \int_{z_b}^{\eta} (\rho u) dz &= \text{①} \left[ \rho u \Big|_{\eta} \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} \int_{z_b}^{\eta} (\rho u u) dz \right] \\ &+ \text{②} \left[ \rho u u \Big|_{z_b} \frac{\partial z_b}{\partial x} - \rho u u \Big|_{\eta} \frac{\partial \eta}{\partial x} + \frac{\partial}{\partial y} \int_{z_b}^{\eta} (\rho u v) dz \right] \\ &+ \rho u v \Big|_{z_b}^{\text{②}} \frac{\partial z_b}{\partial y} - \rho u v \Big|_{\eta}^{\text{①}} \frac{\partial \eta}{\partial y} + \rho u w \Big|_{\eta}^{\text{①}} - \rho u w \Big|_{z_b}^{\text{②}} \end{aligned} \quad (1.2.25)$$

The above expression reduces to the following:

$$\frac{\partial}{\partial t} \int_{z_b}^{\eta} (\rho u) dz + \frac{\partial}{\partial x} \int_{z_b}^{\eta} (\rho u u) dz + \frac{\partial}{\partial y} \int_{z_b}^{\eta} (\rho u v) dz \quad (1.2.26)$$

The following terms are next defined

$$h\bar{u} = (\eta - z_b) \bar{u} = \int_{z_b}^{\eta} u(z) dz, h\bar{v} = (\eta - z_b) \bar{v} = \int_{z_b}^{\eta} v(z) dz \quad (1.2.27)$$

where

$$u(z) = \bar{u} [1 + u'(z)]$$

$$v(z) = \bar{v} [1 + v'(z)]$$

Thus

$$h\bar{u} = \int_{z_b}^{\eta} \bar{u} dz + \int_{z_b}^{\eta} \bar{u} u' dz = h\bar{u} + \bar{u} \int_{z_b}^{\eta} u' dz \quad (1.2.28)$$

$$h\bar{v} = \int_{z_b}^{\eta} \bar{v} dz + \int_{z_b}^{\eta} \bar{v} v' dz = h\bar{v} + \bar{v} \int_{z_b}^{\eta} v' dz \quad (1.2.29)$$

Therefore we must have

$$\int_{z_b}^{\eta} u' dz = \int_{z_b}^{\eta} v' dz = 0 \quad (1.2.30)$$

Rewriting (1.2.26) and employing assumption 8 we obtain

$$\begin{aligned}
\rho \frac{\partial}{\partial t} (\bar{u}h) + \rho \frac{\partial}{\partial x} \int_{z_b}^{\eta} \bar{u} \bar{u} [1 + 2u'(z) + u'(z)^2] dz \\
+ \rho \frac{\partial}{\partial y} \int_{z_b}^{\eta} \bar{u} \bar{v} [1 + u'(z) + v'(z) + u'(z)v'(z)] dz
\end{aligned} \quad (1.2.31)$$

Let

$$\beta = \frac{1}{h} \int_{z_b}^{\eta} \{1 + [u'(z)]^2\} dz = \frac{1}{h} \int_{z_b}^{\eta} [1 + u'(z)v'(z)] dz$$

Noting the depth integral of the product of a bar and primed quantity is zero, we finally obtain

$$\rho \left[ \frac{\partial}{\partial t} (\bar{u}h) + \frac{\partial}{\partial x} (\beta \bar{u} \bar{u} h) + \frac{\partial}{\partial y} (\beta \bar{u} \bar{v} h) \right] \quad (1.2.32)$$

Analogously, one obtains the following expression for the left hand side of the y-motion equation (1.3) after integration over depth

$$\rho \left[ \frac{\partial}{\partial t} (\bar{v}h) + \frac{\partial}{\partial x} (\beta \bar{u} \bar{v} h) + \frac{\partial}{\partial y} (\bar{v} \bar{v} h) \right] \quad (1.2.33)$$

where

$$\beta = \frac{1}{h} \int_{z_b}^{\eta} \{1 + [v'(z)]^2\} dz = \frac{1}{h} \int_{z_b}^{\eta} [1 + u'(z)v'(z)] dz$$

Thus  $\beta$  in (1.2.32) and in (1.2.33) is the same quantity and is usually assumed equal to unity.

Let us now consider the right hand side of the  $x$  and  $y$  motion equations. Considering the  $F_x$  and  $F_y$  terms, we obtain

$$F_x = \Omega v + g_x + G_x \quad F_y = -\Omega u + g_y + G_y \quad (1.2.34)$$

where  $G$  is the tide-generating force,  $\Omega$  is the Coriolis factor,  $\Omega = 2w \sin \phi$  ( $w \equiv$  angular velocity of the earth rotation,  $\phi$  is latitude), and  $g_x$ ,  $g_y$  are the components of gravity in the horizontal. Assume the following:

1.  $g_x$ ,  $G_x \ll \Omega v$ ,
2.  $g_y$ ,  $G_y \ll \Omega u$ ,

then,

$$F_x = \Omega v, \quad F_y = -\Omega u$$

Integrating over the vertical

$$\int_{z_b}^{\eta} \Omega v \, dz = \Omega \bar{v} h \quad \int_{z_b}^{\eta} -\Omega u \, dz = -\Omega \bar{u} h \quad (1.2.35)$$

where  $\bar{u}$ ,  $\bar{v}$  are vertically averaged velocity components, and  $h = \eta - z_b$ .

For a turbulent flow an eddy viscosity  $\varepsilon$  is employed in the place of the dynamic viscosity  $\mu$ . The terms become using  $\varepsilon_h$  and  $\varepsilon_v$  for horizontal and vertical eddy viscosity, respectively:



$$\begin{aligned} \epsilon_h \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \epsilon_v \frac{\partial^2 u}{\partial z^2} \\ \epsilon_h \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \epsilon_v \frac{\partial^2 v}{\partial z^2} \end{aligned} \quad (1.2.36)$$

The horizontal eddy viscosity terms are much smaller than the vertical eddy viscosity terms and have been neglected by some modellers. We consider the terms here in the following manner. If we consider the  $u$  equation and note  $u = \bar{u} + u'$ , integrate over the vertical, and employ Leibniz rule, the following relation is obtained for the  $\epsilon$  terms.

$$\begin{aligned} \int_{z_b}^{\eta} \frac{\partial^2 (\bar{u} + u')}{\partial x^2} dz = \frac{\partial}{\partial x} \int_{z_b}^{\eta} \frac{\partial}{\partial x} (\bar{u} + u') dz \\ + \frac{\partial u}{\partial x} \Big|_{z_b} \frac{\partial z_b}{\partial x} - \frac{\partial u}{\partial x} \Big|_{\eta} \frac{\partial \eta}{\partial x} \end{aligned} \quad (1.2.37)$$

$$\begin{aligned} \int_{z_b}^{\eta} \frac{\partial^2 (\bar{u} + u')}{\partial x^2} dz = \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} \int_{z_b}^{\eta} (\bar{u} + u') dz \right. \\ \left. + u \Big|_{z_b} \frac{\partial z_b}{\partial x} - u \Big|_{\eta} \frac{\partial \eta}{\partial x} \right] + \frac{\partial u}{\partial x} \Big|_{z_b} \frac{\partial z_b}{\partial x} - \frac{\partial u}{\partial x} \Big|_{\eta} \frac{\partial \eta}{\partial x} \end{aligned} \quad (1.2.38)$$

It is assumed that all derivative terms may be neglected, thus

$$\int_{z_b}^{\eta} \frac{\partial^2 (\bar{u} + u')}{\partial x^2} dz = \frac{\partial^2}{\partial x^2} (h\bar{u}) = h \frac{\partial^2 \bar{u}}{\partial x^2} + 2 \frac{\partial h}{\partial x} \frac{\partial \bar{u}}{\partial x} + \bar{u} \frac{\partial^2 h}{\partial x^2} \quad (1.2.39)$$

It is further assumed the second and third terms are negligible. If similar assumptions are made for the other terms in (1.2.36) we obtain

$$\int_{z_b}^{\eta} \epsilon_h \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) dz = \epsilon_h \left[ \frac{\partial^2 (h\bar{u})}{\partial x^2} + \frac{\partial^2 (h\bar{u})}{\partial y^2} \right]$$

$$= \epsilon_h h \left( \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} \right) \quad (1.2.40)$$

$$\int_{z_b}^{\eta} \epsilon_h \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) dz = \epsilon_h \left[ \frac{\partial^2 (h\bar{v})}{\partial x^2} + \frac{\partial^2 (h\bar{v})}{\partial y^2} \right]$$

$$= \epsilon_h h \left( \frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} \right) \quad (1.2.41)$$

These terms are retained in the motion equations and serve to stabilize the numerical approximations. The vertical eddy viscosity terms are integrated over the vertical as follows.

$$\int_{z_b}^{\eta} \epsilon_v \frac{\partial^2 u}{\partial z^2} dz = \epsilon_v \left( \left. \frac{\partial u}{\partial z} \right|_{\eta} - \left. \frac{\partial u}{\partial z} \right|_{z_b} \right) = \tau_{sx} - \tau_{bx} \quad (1.2.42)$$

$$\int_{z_b}^{\eta} \epsilon_v \frac{\partial^2 v}{\partial z^2} dz = \epsilon_v \left( \left. \frac{\partial v}{\partial z} \right|_{\eta} - \left. \frac{\partial v}{\partial z} \right|_{z_b} \right) = \tau_{sy} - \tau_{by} \quad (1.2.43)$$

where  $\tau_{sx}$ ,  $\tau_{sy}$  are surface stresses and  $\tau_{by}$ ,  $\tau_{bx}$  bottom stresses.

Consider the bottom stress,  $\tau_b$ , as follows:

$$\tau_b = C_f \rho \frac{V_f^2}{2}$$

where  $C_f$  is a drag coefficient and  $V_f$  is the fluid velocity. Letting Chézy  $c = \sqrt{2g/C_f}$

obtain:

$$\tau_b = \frac{g}{2} \rho v_f^2 \quad (1.2.44)$$

Resolve  $\tau_b$  along the x and y directions noting  $v_f = \sqrt{\bar{u}^2 + \bar{v}^2}$  to obtain:

$$\tau_{bx} = \frac{\rho g}{2} v_f \bar{u} \quad \tau_{by} = \frac{\rho g}{2} v_f \bar{v} \quad (1.2.45)$$

The surface stress  $\tau_s$  may have a similar form; namely,

$$\tau_s = c'_f \frac{\rho_a v_w^2}{2}$$

where

$c'_f \equiv$  drag coefficient

$\rho_a \equiv$  air density

$v_w \equiv$  wind speed

Assuming the shear stress varies linearly with depth we obtain

$$\frac{\partial \tau}{\partial z} = \frac{\tau_s + \tau_b}{h} = \frac{\tau_s}{h} \left( 1 + \frac{\tau_b}{\tau_s} \right) = \frac{\lambda \tau_s}{h} = \frac{\partial \rho_{wd}}{\partial s} \quad (1.2.46)$$

where

$$\lambda \equiv (\tau_b / \tau_s + 1)$$

$\rho_{wd} \equiv$  pressure intensity produced by the wind

$s \equiv$  distance in the downwind direction

Integrating (1.2.46) over the vertical

$$\int_{z_b}^{\eta} \frac{\partial \tau}{\partial z} dz = \int_{z_b}^{\eta} \frac{c_f' \lambda \rho_a V_w^2}{2h} dz = KV_w^2 \quad (1.2.47)$$

with

$$K = (c_f' \lambda \rho_a)/2$$

If  $\theta$  is the angle between the wind direction and the  $+x$  axis,

$$\tau_{sx} = KV_w^2 \cos \theta \quad (1.2.48)$$

$$\tau_{sy} = KV_w^2 \sin \theta \quad (1.2.49)$$

Assembling our results, we obtain the final expression for the depth integrated motion equations

$$\begin{aligned} \rho \frac{\partial}{\partial t} (\bar{u}h) + \rho \frac{\partial}{\partial x} (\beta \bar{u}^2 h) + \rho \frac{\partial}{\partial y} (\beta \bar{u} \bar{v} h) = \rho \Omega \bar{v} h + h \epsilon_h \left( \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} \right) \\ - h \left( \frac{\partial \rho_a}{\partial x} + \bar{\rho}_g \frac{\partial \eta}{\partial x} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial x} \right) - \frac{\rho g (\bar{u} + \bar{v})^{1/2} \bar{u}}{c^2} + KV_w^2 \cos \theta \end{aligned} \quad (1.2.50)$$

$$\begin{aligned} \rho \frac{\partial}{\partial t} (\bar{v}h) + \rho \frac{\partial}{\partial x} (\beta \bar{u} \bar{v} h) + \rho \frac{\partial}{\partial y} (\beta \bar{v}^2 h) = - \rho \Omega \bar{u} h + h \epsilon_h \left( \frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} \right) \\ - h \left( \frac{\partial \rho_a}{\partial y} + \bar{\rho}_g \frac{\partial \eta}{\partial y} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial y} \right) - \frac{\rho g (\bar{u} + \bar{v})^{1/2} \bar{v}}{c^2} + KV_w^2 \sin \theta \end{aligned} \quad (1.2.51)$$

Setting  $\beta = 1$  and expanding the left-hand side of the above two equations one obtains

$$\begin{aligned}
\rho \left[ h \frac{\partial \bar{u}}{\partial t} + \bar{u} \left( \frac{\partial \eta}{\partial t} - \frac{\partial z}{\partial t} \right)^0 + 2\bar{u}h \frac{\partial \bar{u}}{\partial x} + \overbrace{\left( \frac{\partial \eta}{\partial x} - \frac{\partial z}{\partial x} \right)}^{\partial h / \partial x} \bar{u}^2 + \bar{u}\bar{v} \overbrace{\left( \frac{\partial \eta}{\partial y} - \frac{\partial z}{\partial y} \right)}^{\partial h / \partial y} \right. \\
\left. + h \left( \bar{u} \frac{\partial v}{\partial y} + \bar{v} \frac{\partial \bar{u}}{\partial y} \right) \right] = \rho \left[ h \frac{\partial \bar{u}}{\partial t} + \bar{u} \left( \frac{\partial \eta}{\partial t} + h \frac{\partial \bar{u}}{\partial x} + \bar{u} \frac{\partial h}{\partial x} + \bar{v} \frac{\partial h}{\partial y} + h \frac{\partial v}{\partial y} \right) \right. \\
\left. + h\bar{u} \frac{\partial \bar{u}}{\partial x} + h\bar{v} \frac{\partial \bar{u}}{\partial y} \right] = \rho h \left\{ \frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \frac{\bar{u}}{h} \left[ \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} (\bar{u}h) \right]^0 \right. \\
\left. + \frac{\partial}{\partial y} (\bar{v}h) \right\} = \rho h \frac{D\bar{u}}{Dt} \quad (1.2.52)
\end{aligned}$$

$$\begin{aligned}
\rho \left[ h \frac{\partial \bar{v}}{\partial t} + \bar{v} \left( \frac{\partial \eta}{\partial t} - \frac{\partial z}{\partial t} \right)^0 + 2\bar{v}h \frac{\partial \bar{v}}{\partial y} + \bar{v}^2 \frac{\partial h}{\partial y} + \bar{u}\bar{v} \frac{\partial h}{\partial x} + h \left( \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial x} \right) \right] \\
= \rho \left[ h \frac{\partial \bar{v}}{\partial t} + \bar{v} \left( \frac{\partial \eta}{\partial t} + h \frac{\partial \bar{v}}{\partial y} + \bar{v} \frac{\partial h}{\partial y} + \bar{u} \frac{\partial h}{\partial x} + h \frac{\partial \bar{u}}{\partial x} \right) + h\bar{v} \frac{\partial \bar{v}}{\partial y} + h\bar{u} \frac{\partial \bar{v}}{\partial x} \right] \\
= \rho h \left\{ \frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \frac{\bar{v}}{h} \left[ \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} (\bar{u}h) \right]^0 + \frac{\partial}{\partial y} (\bar{v}h) \right\} \\
= \rho h \frac{D\bar{v}}{Dt} \quad (1.2.53)
\end{aligned}$$

Letting  $\varepsilon_h = \rho\varepsilon$  ( $\varepsilon$  is a kinematic eddy viscosity) and dropping the bar notation we obtain the final form of the equations:

$$\begin{aligned}
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \Omega v + \varepsilon \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g \frac{(u+v)^{1/2}}{c_h^2} + \frac{K}{\rho h} v_w^2 \cos \theta \\
- \frac{1}{\rho} \left( \frac{\partial p_a}{\partial x} + \bar{\rho} g \frac{\partial \eta}{\partial x} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial x} \right) \quad (1.2.54)
\end{aligned}$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\Omega u + \varepsilon \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - g \frac{(u+v)^{1/2}}{c^2 h} + \frac{K}{\rho h} V_w^2 \sin \theta - \frac{1}{\rho} \left( \frac{\partial p_a}{\partial y} + \bar{\rho} g \frac{\partial \eta}{\partial y} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial y} \right) \quad (1.2.55)$$

## 2. Transport Equation

The general transport equation is given for laminar flow as

$$\begin{aligned} \frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y} + w \frac{\partial s}{\partial z} = \frac{\partial}{\partial x} \left( D_x \frac{\partial s}{\partial x} \right) \\ + \frac{\partial}{\partial y} \left( D_y \frac{\partial s}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial s}{\partial z} \right) \end{aligned} \quad (2.1)$$

where

$s \equiv$  concentration of the material of concern

$D_x \equiv$  molecular diffusion coefficient in the  $x$  direction

$D_y \equiv$  molecular diffusion coefficient in the  $y$  direction

$D_z \equiv$  molecular diffusion coefficient in the  $z$  direction

$t, x, y, z, u, v, w$  are as previously defined.

For a turbulent flow, the eddy dispersion is significantly greater than the molecular diffusion. The following analogous formula holds where time averaging over the time scale of the turbulence has been performed.

$$\begin{aligned} \frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y} + w \frac{\partial s}{\partial z} = \frac{\partial}{\partial x} \left( K_x \frac{\partial s}{\partial x} \right) \\ + \frac{\partial}{\partial y} \left( K_y \frac{\partial s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial s}{\partial z} \right) \end{aligned} \quad (2.2)$$

where

$K_x, K_y,$  and  $K_z$  are turbulent eddy dispersion coefficients.

Equation (2.2) may be written in conservation form by adding  $s$  times Equation (1.1) (namely, zero) to the left hand side to obtain

$$\frac{\partial s}{\partial t} + \frac{\partial(us)}{\partial x} + \frac{\partial(vs)}{\partial y} + \frac{\partial(ws)}{\partial z} = \frac{\partial}{\partial x} \left( K_x \frac{\partial s}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial s}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial s}{\partial z} \right) \quad (2.3)$$

This form of the equation is then depth integrated. Considering the left hand side

$$\underbrace{\int_{z_b}^{\eta} \frac{\partial s}{\partial t} dz}_{\textcircled{1}} + \underbrace{\int_{z_b}^{\eta} \frac{\partial(us)}{\partial x} dz}_{\textcircled{2}} + \underbrace{\int_{z_b}^{\eta} \frac{\partial(vs)}{\partial y} dz}_{\textcircled{3}} + \underbrace{\int_{z_b}^{\eta} \frac{\partial(ws)}{\partial z} dz}_{\textcircled{4}} \quad (2.4)$$

Each term is expanded employing Leibniz rule, and the expressions below are obtained

$$\begin{aligned} \textcircled{1} \quad & \frac{\partial}{\partial t} \int_{z_b}^{\eta} s dz + \frac{\partial z_b}{\partial t} s \bigg|_{\substack{z \\ \text{bottom rigid}}} - \frac{\partial \eta}{\partial t} s \bigg|_{\eta} \\ \textcircled{2} \quad & \frac{\partial}{\partial x} \int_{z_b}^{\eta} us dz + \frac{\partial z_b}{\partial x} (us) \bigg|_{z_b} - \frac{\partial \eta}{\partial x} (us) \bigg|_{\eta} \\ \textcircled{3} \quad & \frac{\partial}{\partial y} \int_{z_b}^{\eta} vs dz + \frac{\partial z_b}{\partial y} (vs) \bigg|_{z_b} - \frac{\partial \eta}{\partial y} (vs) \bigg|_{\eta} \\ \textcircled{4} \quad & ws \bigg|_{\eta} - ws \bigg|_{z_b} \end{aligned} \quad (2.5)$$

Note

$$s \left( u \frac{\partial z}{\partial x} + v \frac{\partial z}{\partial y} - w \right) \Big|_{z_b} = 0$$

and

$$s \left( w - \frac{\partial \eta}{\partial t} - u \frac{\partial \eta}{\partial x} - v \frac{\partial \eta}{\partial y} \right) \Big|_{\eta} = 0$$

from kinematic considerations.

The left hand side (2.4) then reduces to the following expression

$$\frac{\partial}{\partial t} \int_{z_b}^{\eta} s \, dz + \frac{\partial}{\partial x} \int_{z_b}^{\eta} (us) \, dz + \frac{\partial}{\partial y} \int_{z_b}^{\eta} (vs) \, dz \quad (2.6)$$

Let

$$s = \bar{s} + s' , \quad v = \bar{v} + v' , \quad u = \bar{u} + u' , \quad h = \eta - z$$

where

$$\int_{z_b}^{\eta} s' \, dz = \int_{z_b}^{\eta} v' \, dz = \int_{z_b}^{\eta} u' \, dz = 0 \quad (2.7)$$

Each of the three terms in (2.6) is expanded to yield

$$\frac{\partial}{\partial t} \int_{z_b}^{\eta} s \, dz = \frac{\partial}{\partial t} (h\bar{s}) \quad (2.8)$$

$$\begin{aligned} \frac{\partial}{\partial x} \int_{z_b}^{\eta} (us) \, dz &= \frac{\partial}{\partial x} \int_{z_b}^{\eta} (\bar{u}\bar{s} + u'\bar{s} + s'\bar{u} + u's') \, dz \\ &= \frac{\partial}{\partial x} \left[ (h\bar{u}\bar{s}) + h(u's')_h \right] \end{aligned} \quad (2.9)$$



where

$$\int_{z_b}^{\eta} u's' dz = h(u's')_h$$

$$\begin{aligned} \frac{\partial}{\partial y} \int_{z_b}^{\eta} (vs) dz &= \frac{\partial}{\partial y} \int_{z_b}^{\eta} (\bar{v}\bar{s} + v'\bar{s} + s'\bar{v} + v's') dz \\ &= \frac{\partial}{\partial y} \left[ (h\bar{v}\bar{s}) + h(v's')_h \right] \end{aligned} \quad (2.10)$$

where

$$\int_{z_b}^{\eta} v's' dz = h(v's')_h$$

For the left hand side we then finally obtain

$$\frac{\partial}{\partial t} (h\bar{s}) + \frac{\partial}{\partial x} (h\bar{u}\bar{s}) + \frac{\partial}{\partial y} (h\bar{v}\bar{s}) + \frac{\partial}{\partial x} \left[ h(u's')_h \right] + \frac{\partial}{\partial y} \left[ h(v's')_h \right] \quad (2.11)$$

Consider now the right hand side of (2.2). As previously mentioned, the turbulent dispersion coefficients are developed from time averaging the turbulence. Specifically,

$$\frac{\partial}{\partial x} \left( K_x \frac{\partial s}{\partial x} \right) = - \frac{\partial}{\partial x} (u''s'')_t \quad (2.12)$$

$$\frac{\partial}{\partial y} \left( K_y \frac{\partial s}{\partial y} \right) = - \frac{\partial}{\partial y} (v''s'')_t \quad (2.13)$$

$$\frac{\partial}{\partial z} \left( K_z \frac{\partial s}{\partial z} \right) = - \frac{\partial}{\partial z} (w''s'')_t \quad (2.14)$$

where  $t$  denotes time averaging and the double prime denotes a time fluctuation. The terms on the right hand side can now be integrated employing Leibniz rule to obtain

$$\int_{z_b}^{\eta} \frac{\partial}{\partial x} (u''s'')_t dz = \frac{\partial}{\partial x} \int_{z_b}^{\eta} (u''s'')_t dz + (u''s'')_t \bigg|_{z_b} \frac{\partial z_b}{\partial x} - (u''s'')_t \bigg|_{\eta} \frac{\partial \eta}{\partial x} \quad (2.15)$$

$$\int_{z_b}^{\eta} \frac{\partial}{\partial y} (v''s'')_t dz = \frac{\partial}{\partial y} \int_{z_b}^{\eta} (v''s'')_t dz + (v''s'')_t \bigg|_{z_b} \frac{\partial z_b}{\partial y} - (v''s'')_t \bigg|_{\eta} \frac{\partial \eta}{\partial y} \quad (2.16)$$

$$\int_{z_b}^{\eta} \frac{\partial}{\partial z} (w''s'')_t dz = (w''s'')_t \bigg|_{\eta} - (w''s'')_t \bigg|_{z_b} \quad (2.17)$$

If we assume all terms in the above three relations are zero except the integrals, the last equation is removed from further consideration. Additionally if we bring the last two terms in (2.11) to the right hand side we obtain

$$\begin{aligned} \frac{\partial}{\partial t} (h\bar{s}) + \frac{\partial}{\partial x} (h\bar{v}s) + \frac{\partial}{\partial y} (h\bar{w}s) = & - \frac{\partial}{\partial x} \left\{ h \left[ (u's')_h + (u''s'')_{th} \right] \right\} \\ & - \frac{\partial}{\partial y} \left\{ h \left[ (v's')_h + (v''s'')_{th} \right] \right\} \end{aligned} \quad (2.18)$$

where

$$h(u''s'')_{th} = \int_b^h (u''s'')_t dz \quad \text{and} \quad h(v''s'')_{th} = \int_{z_b}^{\eta} (v''s'')_t dz$$

Letting, after Pritchard [3],

$$(u's')_h + (u''s'')_{th} = -K_x^* \frac{\partial \bar{s}}{\partial x} \quad (2.19)$$

$$(v's')_h + (v''s'')_{th} = -K_y^* \frac{\partial \bar{s}}{\partial y} \quad (2.20)$$

one finally obtains, dropping the bar notation, the vertically integrated form of the transport equation as given below.

$$\frac{\partial}{\partial t} (hs) + \frac{\partial}{\partial x} (hus) + \frac{\partial}{\partial y} (hvs) = \frac{\partial}{\partial x} \left( hK_x^* \frac{\partial s}{\partial x} \right) + \frac{\partial}{\partial y} \left( hK_y^* \frac{\partial s}{\partial y} \right) \quad (2.21)$$

### 3. Equation of State

The density of water is a complex function of temperature, pressure, and salinity. The Tumlirz equation is used to define this relationship as follows

$$(p + p_o) (v - v_o) = \lambda \quad (3.1)$$

where

$p \equiv$  pressure in atmospheres

$p_o \equiv$  baseline pressure in atmosphere

$v \equiv$  specific volume in ml/gm

$v_o \equiv$  baseline specific volume in ml/gm

$\lambda \equiv$  constant [(ml/gm) atm]

and  $\lambda$ ,  $p_o$ , and  $v_o$  are functions of temperature and salinity. Eckart has reported the following relationships

$$\lambda = 1779.5 + 11.25T - 0.0745T^2 - (3.8 + 0.01T)S$$

$$v_o = 0.698$$

$$p_o = 5890 + 38T - 0.375T^2 + 3S$$

Since water is only slightly compressible, we may neglect pressure effects in (3.1) by setting  $p = 0$  and obtain

$$\rho = \frac{1}{v} = \frac{p_o}{\lambda + v_o p_o} \quad (3.2)$$

where  $\rho$  is the density in (gm/ml). In (1.2.54) and (1.2.55)  $\bar{\rho}$  is given as in (3.2) with  $\rho$  set equal to 1(gm/ml). In order to describe temperature an equation similar to (2.21) must be considered. It is proposed at this time to specify a temperature distribution directly from measured data rather than approximate (2.21) for temperature.

#### 4. Compilation of the Complete Set of Equations

Relations (1.1.9) (Continuity), (1.2.54) (x-motion), (1.2.55) (y-motion), (2.21) (Salinity transport), and (3.2) (State), constitute the complete set of density coupled equations.

In cases where density effects may be neglected within the hydrodynamics, the system assumes an uncoupled form with the following format. Equation (1.1.9) remains unchanged. Equation (3.2), the state equation, is no longer needed. The pressure gradient terms in (1.2.54) and (1.2.55) reduce to the following relations:

$$\frac{\partial p_a}{\partial x} + \bar{\rho}g \frac{\partial \eta}{\partial x} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial x} \rightarrow \frac{\partial p_a}{\partial x} + \rho g \frac{\partial \eta}{\partial x} \quad (4.1)$$

$$\frac{\partial p_a}{\partial y} + \bar{\rho}g \frac{\partial \eta}{\partial y} + \frac{gh}{2} \frac{\partial \bar{\rho}}{\partial y} \rightarrow \frac{\partial p_a}{\partial y} + \rho g \frac{\partial \eta}{\partial y} \quad (4.2)$$

It is proposed to initially consider the uncoupled system of equations. In this manner the suitability of the numerical approximation to (2.21) can be assessed directly.

### PART III: LITERATURE REVIEW

The transport equation exhibits both hyperbolic and parabolic characteristics. For convection much larger than dispersion as is the case in estuarine systems, the equation's character becomes predominantly hyperbolic. It is this property which makes numerical approximation difficult. In order to most effectively develop a numerical approximation the Water Resources Research, Journal of the Hydraulics Division, Journal of Waterways Harbors and Coastal Engineering Division, International Journal for Numerical Methods In Engineering, Advances in Water Resources, and Applied Mathematical Modeling were searched over the period of holdings at the Waterways Experiment Station Library. Additional references were also obtained from the Journal of Computational Physics.

The numerical approximation of the transport equation is an active research area within each of three major numerical analysis disciplines: finite difference, finite element, and method of characteristics. Review was limited to finite difference techniques. The following eight major methods presented in Table I were investigated and are reported in turn in detail. Additional techniques found in the literature are briefly outlined along with practical considerations in selecting a numerical method.

1. Sheng Work at Aeronautical Research Associates of Princeton (ARAP)

Sheng [4] considers the following equation

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} + \frac{\partial wc}{\partial z} = 0 \quad (1.1)$$

Table I  
Major Numerical Methods

<u>Method</u>	<u>Advantages</u>	<u>Disadvantages</u>
1. Centered space differences with ARAP smoothing	Consistent with present hydrodynamics (ADI)	Potential for negative concentrations
2. Flux-Corrected Transport	Positivity of concentrations	Two schemes must be implemented (higher and lower order)
3. Holly-Preissmann Scheme	Explicit (coding may be simpler)	Explicit time step limit. Not developed for two dimensions
4. Method of Second Moments	Explicit (coding may be simpler)	Diffusion not considered. Explicit time step limit.
5. Balanced Expansion Technique	Phase error may be systematically reduced	Explicit and diffusion time step limit. Not developed for two dimensions.
6. Stone and Brian Technique	Consistent with present hydrodynamics (ADI)	Potential for negative concentrations
7. Gray and Pinder	Consistent with present hydrodynamics (ADI)	Potential for negative concentrations
8. Leendertse Scheme	Consistent with present hydrodynamics (ADI)	Potential for negative concentrations

The following finite difference form of (1.1) is considered.

$$c_{i,k}^{n+1} = c_{i,k}^n - \frac{\Delta t}{\Delta x \Delta z} (f_R - f_L + g_T - g_B) \quad (1.2)$$

where

$f_R \equiv$  right flux for grid cell surrounding  $c_{i,k}$

$f_L \equiv$  left flux for grid cell surrounding  $c_{i,k}$

$g_T \equiv$  top flux for grid cell surrounding  $c_{i,k}$

$g_B \equiv$  bottom flux for grid cell surrounding  $c_{i,k}$

The quantities in (1.2) are indicated in Figure 1. Several approximations are presented for  $f_R$ ,  $f_L$ ,  $g_T$ , and  $g_B$  based upon several alternative difference schemes. These are presented in turn below.

#### UPWIND SCHEME

$$f_R = \begin{cases} u_{i,k} \cdot c_{i+1,k}(\Delta z) & u_{i,k} < 0 \\ u_{i,k} \cdot c_{i,k}(\Delta z) & u_{i,k} > 0 \end{cases} \quad (1.3a)$$

$$f_L = \begin{cases} u_{i-1,k} \cdot c_{i,k}(\Delta z) & u_{i-1,k} < 0 \\ u_{i-1,k} \cdot c_{i-1,k}(\Delta z) & u_{i-1,k} > 0 \end{cases} \quad (1.3b)$$

$$g_T = \begin{cases} w_{i,k} \cdot c_{i,k+1}(\Delta x) & w_{i,k} < 0 \\ w_{i,k} \cdot c_{i,k}(\Delta x) & w_{i,k} > 0 \end{cases} \quad (1.3c)$$

$$g_B = \begin{cases} w_{i,k-1} \cdot c_{i,k}(\Delta x) & w_{i,k-1} < 0 \\ w_{i,k-1} \cdot c_{i,k-1}(\Delta x) & w_{i,k-1} > 0 \end{cases} \quad (1.3d)$$



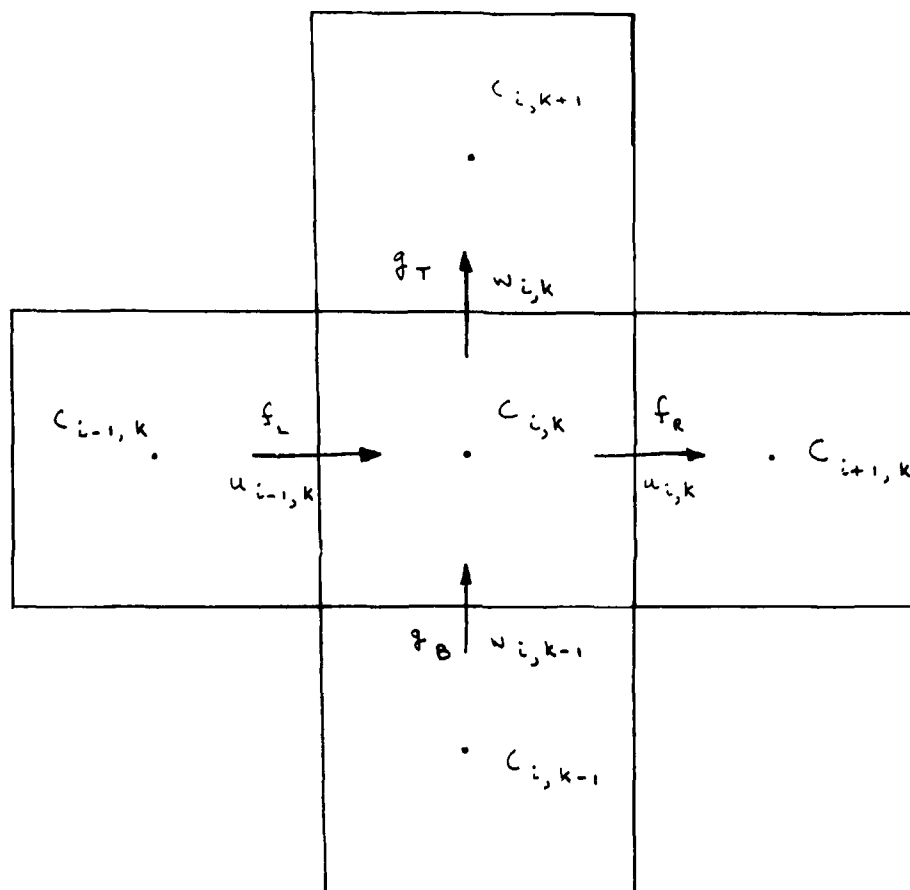


Figure 1. Notation for presentation of Sheng schemes

Let us consider the case  $u_{i,k} > 0$ ,  $u_{i-1,k} > 0$  and  $w_{i,k}$ ,  $w_{i,k-1} > 0$  to illustrate the final form by substituting the above relations under these conditions into (1.2) above:

$$\begin{aligned} \frac{c_{i,k}^{n+1} - c_{i,k}^n}{\Delta t} = & - \frac{(u_{i,k} c_{i,k} - u_{i-1,k} c_{i-1,k})}{\Delta x} \\ & - \frac{(w_{i,k} c_{i,k} - w_{i,k-1} c_{i,k-1})}{\Delta z} \end{aligned} \quad (1.4)$$

If  $u_{i,k} = u_{i-1,k}$  and  $w_{i,k} = w_{i-1,k}$ , then the above equation reduces to the following form:

$$\frac{c_{i,k}^{n+1} - c_{i,k}^n}{\Delta t} = - \frac{u_{i,k}}{\Delta x} (c_{i,k} - c_{i-1,k}) - \frac{w_{i,k}}{\Delta z} (c_{i,k} - c_{i,k-1}) \quad (1.5)$$

and the space differences are only first order accurate. In computation, an artificial (numerical) dispersion is introduced.

#### CENTRAL DIFFERENCE SCHEME

$$f_R = u_{i,k} \frac{(c_{i+1,k} + c_{i,k})}{2} (\Delta z) \quad (1.6a)$$

$$f_L = u_{i-1,k} \frac{(c_{i-1,k} + c_{i,k})}{2} (\Delta z) \quad (1.6b)$$

$$g_T = w_{i,k} \frac{(c_{i,k} + c_{i,k+1})}{2} (\Delta x) \quad (1.6c)$$

$$g_B = w_{i,k-1} \frac{(c_{i,k} + c_{i,k-1})}{2} (\Delta x) \quad (1.6d)$$

Substituting the above relations in (1.2) obtain

$$\begin{aligned}
c_{i,k}^{n+1} = c_{i,k}^n - \frac{\Delta t}{\Delta x} \left[ u_{i,k} \frac{(c_{i+1,k} + c_{i,k})}{2} - u_{i-1,k} \frac{(c_{i,k} + c_{i-1,k})}{2} \right] \\
- \frac{\Delta t}{\Delta z} \left[ w_{i,k} \frac{(c_{i,k} + c_{i,k+1})}{2} - w_{i,k-1} \frac{(c_{i,k} + c_{i,k-1})}{2} \right]
\end{aligned} \quad (1.7)$$

Note if  $u_{i,k} = u_{i-1,k}$  and  $w_{i,k} = w_{i,k-1}$ , then (1.7) becomes,

$$\frac{c_{i,k}^{n+1} - c_{i,k}^n}{\Delta t} = - u_{i,k} \frac{(c_{i+1,k} - c_{i-1,k})}{2\Delta x} - w_{i,k} \frac{(c_{i,k+1} - c_{i,k-1})}{2\Delta z} \quad (1.8)$$

We note in (1.8) above that the spatial differences are centered in the x and z directions and are thus second order accurate. Although these forms are more accurate than upwind differencing, an oscillatory behavior has been observed when they are used to propagate steep fronts. Negative concentrations are thereby obtained.

#### COMBINED UPWIND AND CENTRAL DIFFERENCE

In order to avoid negative concentrations but reduce the smearing effect, the following combined scheme has been suggested.

$$f_R = \left\{ \begin{array}{lll} u_{i,k} c_{i,k} (\Delta z) & u_{i,k} > 0 & c_{i,k} < c_{i+1,k} \\ u_{i,k} \frac{(c_{i,k} + c_{i+1,k})}{2} (\Delta z) & u_{i,k} > 0 & c_{i,k} > c_{i+1,k} \\ u_{i,k} c_{i+1,k} (\Delta z) & u_{i,k} < 0 & c_{i,k} > c_{i+1,k} \\ u_{i,k} \frac{(c_{i,k} + c_{i+1,k})}{2} (\Delta z) & u_{i,k} < 0 & c_{i,k} < c_{i+1,k} \end{array} \right\} \quad (1.9a)$$

$$f_L = \left\{ \begin{array}{lll} u_{i-1,k} c_{i-1,k} (\Delta z) & u_{i-1,k} > 0 & c_{i-1,k} < c_{i,k} \\ u_{i-1,k} \frac{(c_{i-1,k} + c_{i,k})}{2} (\Delta z) & u_{i-1,k} > 0 & c_{i-1,k} > c_{i,k} \\ u_{i-1,k} c_{i,k} (\Delta z) & u_{i-1,k} < 0 & c_{i-1,k} > c_{i,k} \\ u_{i-1,k} \frac{(c_{i,k} + c_{i-1,k})}{2} (\Delta z) & u_{i-1,k} < 0 & c_{i-1,k} < c_{i,k} \end{array} \right\} \quad (1.9b)$$

Analogous expressions hold for  $g_T$  and  $g_B$ . This scheme is similar to second upwind differencing and uses the central difference approximations as often as possible. Lower order differencing (first upwind) is employed as necessary to eliminate negative concentrations. The effective advective concentration employed in an outgoing flux is always less than or equal to the concentration of the cell providing the flux.

#### CENTRAL DIFFERENCE SCHEME WITH SPATIAL SMOOTHING

A smoothing scheme developed by Sheng was employed to the central difference scheme (1.7). It appears in most instances negative concentrations may be prevented. However, it is highly desirable to avoid all negative concentrations.

The smoothing scheme examines the solution surface in both coordinate directions, independently, and determines whether oscillations are short or long wave phenomena. Short wave oscillations are smoothed.

The smoothing procedure is as follows for  $v_j$ .

If

$$\Delta_R + \Delta_L \geq \mu \Delta_T \quad (1.10)$$

where

$$\Delta_R = |v_{j+1} - v_j| / \Delta x$$

$$\Delta_L = |v_j - v_{j-1}| / \Delta x$$

$$\Delta_T = |v_{j+1} - v_{j-1}| / 2\Delta x$$

$$\mu \geq 2$$

then the following curvature check is performed.

If

$$\Delta^2 \times \Delta_R^2 < 0 \quad \text{or} \quad \Delta^2 \times \Delta_L^2 < 0 \quad (1.11)$$

where

$$\Delta^2 = (v_{j+1} + v_{j-1} - 2v_j) / \Delta x^2$$

$$\Delta_R^2 = (v_{j+2} + v_j - 2v_{j+1}) / \Delta x^2$$

$$\Delta_L^2 = (v_j + v_{j-2} - 2v_{j-1}) / \Delta x^2$$

then smoothing is applied in the following manner.

$$\hat{v}_j = v_j + \beta(v_{j+1} + v_{j-1} - 2v_j) \quad (1.12)$$

where  $\hat{v}_j$  is the smoothed value for  $v_j$  and  $\beta$  is a positive constant. In practice, tests have suggested  $\mu = 4$  and  $\beta = 1/4$  are the best values to employ in this smoothing procedure.

#### FLUX-CORRECTED-TRANSPORT (FCT) SCHEME

This method was originally developed by Boris and Book [6]. It has been subsequently improved and generalized by Zalesak [7]. It is a two step method, first involving a low order calculation and then a correction to a higher order. The upwind scheme is used to compute the first order result

$$c_{i,k}^{td} = c_{i,k}^n - \frac{\Delta t}{\Delta x \Delta z} \left( f_R^1 - f_L^1 + g_T^1 - g_B^1 \right) \quad (1.13)$$

where  $c_{i,k}^{td}$  is the first order (transported and diffused) concentration. A higher order scheme, e.g., the central difference scheme, can be applied to compute higher order fluxes  $f_R^2$ ,  $f_L^2$ ,  $g_T^2$ , and  $g_B^2$ . Antidiffusive fluxes are then defined as

$$\begin{aligned} A_R &= f_R^2 - f_R^1 \\ A_L &= f_L^2 - f_L^1 \\ A_T &= g_T^2 - g_T^1 \\ A_B &= g_B^2 - g_B^1 \end{aligned} \quad (1.14)$$

It is these antidiffusive fluxes which are limited in the Zalesak [7] procedure such that

$$\begin{aligned} A_R^c &= A_R \cdot D_{i+1/2,k} & 0 \leq D_{i+1/2,k} \leq 1 \\ A_L^c &= A_L \cdot D_{i-1/2,k} & 0 \leq D_{i-1/2,k} \leq 1 \\ A_T^c &= A_T \cdot D_{i,k+1/2} & 0 \leq D_{i,k+1/2} \leq 1 \\ A_B^c &= A_B \cdot D_{i,k-1/2} & 0 \leq D_{i,k-1/2} \leq 1 \end{aligned} \quad (1.15)$$

Finally

$$c_{i,k}^{n+1} = c_{i,k}^{td} - \frac{\Delta t}{\Delta x \Delta z} \left( A_R^c - A_L^c + A_T^c - A_B^c \right) \quad (1.16)$$

The determination of the  $D$  coefficients will be presented subsequently.

## 2. Fully Multidimensional Flux-Corrected Transport Algorithms for Fluids

In this article, Zalesak [7] develops a new flux limiter which generalizes to multidimensional problems. The new flux limiter in one dimension is shown to exhibit superior characteristics over the original limiter.

Zalesak considers the two-dimensional problem in the following fashion. Consider

$$w_{i,j}^{Ltd} = w_{i,j}^n - (\Delta x_{ij} \Delta y_{ij})^{-1} \left( F_{i+1/2,j}^L - F_{i-1/2,j}^L + F_{i,j+1/2}^L - F_{i,j-1/2}^L \right) \quad (2.1)$$

and

$$w_{i,j}^{Htd} = w_{i,j}^n - (\Delta x_{ij} \Delta y_{ij})^{-1} \left( F_{i+1/2,j}^H - F_{i-1/2,j}^H + F_{i,j+1/2}^H - F_{i,j-1/2}^H \right) \quad (2.2)$$

where  $w_{i,j}^{Ltd}$  represents the lower order transported and diffused solution and  $w_{i,j}^{Htd}$  the higher order solution. We observe that the difference between the time advancement may be written as

$$w_{i,j}^{Htd} - w_{i,j}^{Ltd} = - (\Delta x_{i,j} \Delta y_{i,j})^{-1} \left[ \left( F_{i+1/2,j}^H - F_{i+1/2,j}^L \right) - \left( F_{i-1/2,j}^H - F_{i-1/2,j}^L \right) + \left( F_{i,j+1/2}^H - F_{i,j+1/2}^L \right) - \left( F_{i,j-1/2}^H - F_{i,j-1/2}^L \right) \right] \quad (2.3)$$

Note this difference is written as an array of fluxes between different grid points and is the condition required to implement flux corrected transport.

Flux-corrected transport is implemented in the following fashion using implicit difference schemes for  $w_{i,j}^{Ltd}$  and  $w_{i,j}^{Htd}$  :

1. Compute  $w_{i,j}^{Ltd}$  from (2.1) above
2. Calculate  $F^L(w_{i,j}^n, w_{i,j}^{Ltd})$
3. Compute  $w_{i,j}^{Htd}$  from (2.2) above
4. Calculate  $F^H(w_{i,j}^n, w_{i,j}^{Htd})$
5. Determine the antidiffusive fluxes  $F^H - F^L$  as in (2.3) above
6. Limit these antidiffusive fluxes as follows

$$\begin{aligned} A_{i+1/2,j}^c &= A_{i+1/2,j} c_{i+1/2,j} & 0 \leq c_{i+1/2,j} \leq 1 \\ A_{i,j+1/2}^c &= A_{i,j+1/2} c_{i,j+1/2} & 0 \leq c_{i,j+1/2} \leq 1 \end{aligned} \quad (2.4)$$

7. Apply the limited antidiffusive fluxes:

$$\begin{aligned} w_{i,j}^{n+1} &= w_{i,j}^{Ltd} - (\Delta x_{ij} \Delta y_{ij})^{-1} (A_{i+1/2,j}^c - A_{i-1/2,j}^c \\ &\quad + A_{i,j+1/2}^c - A_{i,j-1/2}^c) \end{aligned} \quad (2.5)$$

The crucial step in the above process is Step 6, the flux-limiting stage. The following quantities are computed;

$$\begin{aligned} P_{i,j}^+ &= \text{the sum of all antidiffusive fluxes into grid point } (i,j) \\ &= \max(0, A_{i-1/2,j}) - \min(0, A_{i+1/2,j}) \\ &\quad + \max(0, A_{i,j-1/2}) - \min(0, A_{i,j+1/2}) \end{aligned} \quad (2.6)$$



$$Q_{i,j}^+ = (w_{i,j}^{\max} - w_{i,j}^{\text{Ltd}}) (\Delta x_{ij} \Delta y_{ij}) \quad (2.7)$$

$$R_{i,j}^+ = \begin{cases} \min(1, Q_{i,j}^+ / P_{i,j}^+) & P_{i,j}^+ > 0 \\ 0 & P_{i,j}^+ = 0 \end{cases} \quad (2.8)$$

and

$P_{i,j}^-$  = the sum of all antidiffusive fluxes out of grid point (i,j)

$$\begin{aligned} &= \max(0, A_{i+1/2,j}) - \min(0, A_{i-1/2,j}) \\ &\quad + \max(0, A_{i,j+1/2}) - \min(0, A_{i,j-1/2}) \end{aligned} \quad (2.9)$$

$$Q_{i,j}^- = (w_{i,j}^{\text{Ltd}} - w_{i,j}^{\min}) (\Delta x_{i,j} \Delta y_{i,j}) \quad (2.10)$$

$$R_{i,j}^- = \begin{cases} \min(1, Q_{i,j}^- / P_{i,j}^-) & P_{i,j}^- > 0 \\ 0 & P_{i,j}^- = 0 \end{cases} \quad (2.11)$$

The limiting coefficients are then given by

$$c_{i+1/2,j} = \begin{cases} \min(R_{i+1,j}^+, R_{i,j}^-) & A_{i+1/2,j} \geq 0 \\ \min(R_{i,j}^+, R_{i+1,j}^-) & A_{i+1/2,j} < 0 \end{cases} \quad (2.12)$$

$$c_{i,j+1/2} = \begin{cases} \min(R_{i,j+1}^+, R_{i,j}^-) & A_{i,j+1/2} \geq 0 \\ \min(R_{i,j}^+, R_{i,j+1}^-) & A_{i,j+1/2} < 0 \end{cases} \quad (2.13)$$

Prior to determining these quantities the following procedures are employed.

$$\begin{aligned} A_{i+1/2,j} = 0 & \quad \text{for} \quad A_{i+1/2,j} (w_{i+1,j}^{Ltd} - w_{i,j}^{Ltd}) < 0 \\ & \text{and either} \quad A_{i+1/2,j} (w_{i+2,j}^{Ltd} - w_{i+1,j}^{Ltd}) < 0 \\ & \quad \text{or} \quad A_{i+1/2,j} (w_{i,j}^{Ltd} - w_{i-1,j}^{Ltd}) < 0 \end{aligned} \quad (2.14)$$

$$\begin{aligned} A_{i,j+1/2} = 0 & \quad \text{for} \quad A_{i,j+1/2} (w_{i,j+1}^{Ltd} - w_{i,j}^{Ltd}) < 0 \\ & \text{and either} \quad A_{i,j+1/2} (w_{i,j+2}^{Ltd} - w_{i,j+1}^{Ltd}) < 0 \\ & \quad \text{or} \quad A_{i,j+1/2} (w_{i,j}^{Ltd} - w_{i,j-1}^{Ltd}) < 0 \end{aligned} \quad (2.15)$$

$$w_{i,j}^a = \max(w_{i,j}^n, w_{i,j}^{Ltd}) \quad (2.16)$$

$$w_{i,j}^b = \min(w_{i,j}^n, w_{i,j}^{Ltd}) \quad (2.17)$$

$$w_{i,j}^{\max} = \max(w_{i-1,j}^a, w_{i,j}^a, w_{i+1,j}^a, w_{i,j-1}^a, w_{i,j+1}^a) \quad (2.18)$$

$$w_{i,j}^{\min} = \min(w_{i-1,j}^b, w_{i,j}^b, w_{i+1,j}^b, w_{i,j-1}^b, w_{i,j+1}^b) \quad (2.19)$$

Zalesak notes that while the solution will be kept between  $w^{\min}$  and  $w^{\max}$  monotonicity in one coordinate direction in rare cases may be

violated. Additional, more stringent limitations are given to prevent this occurrence but will not be presented here.

### 3. Holly-Preissmann Scheme

In developing the scheme the following one-dimensional advection equation is considered for constant velocity by Holly and Preissmann [8]

$$\frac{\partial c(x,t)}{\partial t} + u(x,t) \frac{\partial c(x,t)}{\partial x} = 0 \quad (3.1)$$

where

$c(x,t) \equiv$  concentration at  $x$  for time  $t$

$u(x,t) = u_0$  a constant velocity

For this case, the formal solution to (3.1) becomes

$$c(x, t + \tau) = c(x - u_0 \tau, t) \quad (3.2)$$

Therefore the concentration at  $x$  for time  $t + \tau$  is determined from a knowledge of the concentration for time  $t$  at  $x - u_0 \tau$ . This forms the basis for the development of many explicit direct calculation methods. Holly and Preissmann consider the situation shown in Figure 2.

In order to determine  $c_A^n$  an interpolation procedure is needed.

In this scheme information at only the two adjacent grid points is used.

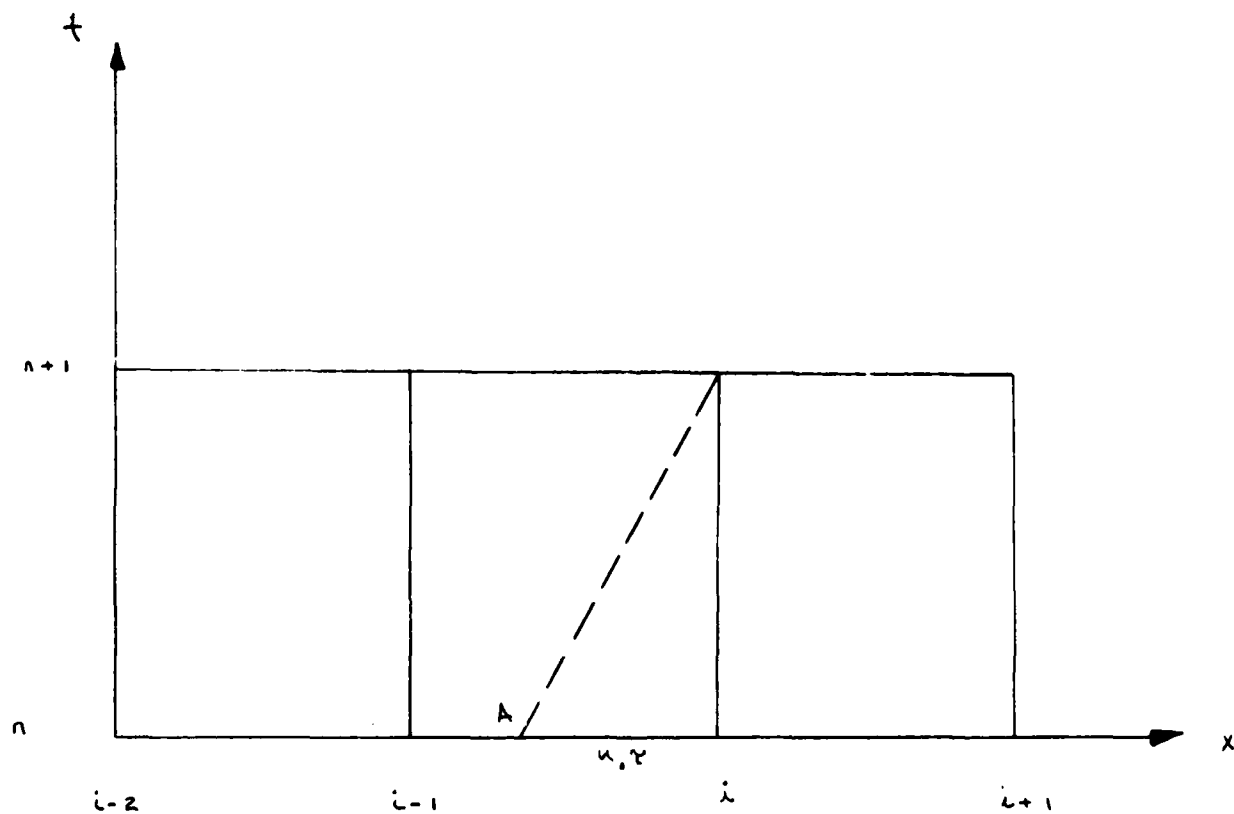
Knowledge of  $c_i^n$ ,  $c_{i-1}^n$  and  $cx_i^n$ ,  $cx_{i-1}^n$  are employed, where

$cx_i^n = \partial c / \partial x$  at  $x = x_i$ ,  $t = t_n$ .

A dimensionless argument  $\alpha$ , known as the Courant number, is defined:

$$\alpha = \frac{u_0 \tau}{x_i - x_{i-1}} \quad (3.3)$$

Letting  $u_0 \tau = x$ , a general distance measured from  $x_i$  to  $x_{i-1}$ ,



$$C_i^{n+1} = C_A^n$$

Figure 2. Holly-Preissmann scheme notation

$$\frac{d\alpha}{dx} = (x_i - x_{i-1})^{-1} \quad \text{and} \quad \frac{dy}{dx} = \frac{dy}{d\alpha} \frac{d\alpha}{dx} = \frac{dy}{d\alpha} (x_i - x_{i-1})^{-1} \quad (3.4)$$

The following interpolating polynomial is considered.

$$y(\alpha) = A\alpha^3 + B\alpha^2 + D\alpha + E \quad (3.5a)$$

$$y(0) = c_i^n = E, \quad y(1) = c_{i-1}^n = A + B + D + E \quad (3.5b)$$

$$\dot{y}(\alpha) = \frac{(3A\alpha^2 + 2B\alpha + D)}{(x_i - x_{i-1})} \quad (3.6a)$$

$$\dot{y}(0) = cx_i^n = \frac{D}{(x_i - x_{i-1})}, \quad \dot{y}(1) = \frac{(3A + 2B + D)}{(x_i - x_{i-1})} = cx_{i-1}^n \quad (3.6b)$$

Equations (3.5b) and (3.6b) are employed to solve for A, B, D, and E. We note E and D are available directly; namely,

$$E = c_i^n, \quad D = (x_i - x_{i-1}) cx_i^n \quad (3.7)$$

From  $y(1)$ , we obtain

$$A = -B + c_{i-1}^n - (x_i - x_{i-1}) cx_i^n - c_i^n \quad (3.8)$$

Substituting in  $\dot{y}(1)$ , we obtain

$$\begin{aligned} cx_{i-1}^n (x_i - x_{i-1}) = & -3B + 3(c_{i-1}^n - c_i^n) - 3(x_i - x_{i-1}) cx_i^n \\ & + 2B + (x_i - x_{i-1}) cx_i^n \end{aligned} \quad (3.9)$$

$$B = 3(c_{i-1}^n - c_i^n) - (2cx_i^n + cx_{i-1}^n)(x_i - x_{i-1}) \quad (3.10)$$

Substituting B into (3.8) we obtain

$$A = -2(c_{i-1}^n - c_i^n) + (cx_i^n + cx_{i-1}^n)(x_i - x_{i-1}) \quad (3.11)$$

Substituting these results into (3.5a), we obtain

$$y(\alpha) = \left[ (cx_i^n + cx_{i-1}^n)(x_i - x_{i-1}) - 2(c_{i-1}^n - c_i^n) \right] \alpha^3 + \left[ 3(c_{i-1}^n - c_i^n) - (2cx_i^n + cx_{i-1}^n)(x_i - x_{i-1}) \right] \alpha^2 + cx_i^n(x_i - x_{i-1})\alpha + c_i^n \quad (3.12)$$

Collecting terms (3.12),  $y(\alpha)$  is rewritten as

$$y(\alpha) = (-2\alpha^3 + 3\alpha^2) c_{i-1}^n + (2\alpha^3 - 3\alpha^2 + 1) c_i^n + (\alpha^3 - \alpha^2)(x_i - x_{i-1}) cx_{i-1}^n + (\alpha^3 - 2\alpha^2 + \alpha)(x_i - x_{i-1}) cx_i^n \quad (3.13)$$

Thus we have

$$c_i^{n+1} = y(\alpha) \quad (3.14)$$

In order to advance the solution in time the concentration derivative also must be determined. For the constant velocity case, differentiating the transport equation with respect to  $x$  and interchanging the order of the  $x$  and  $t$  derivatives

$$\frac{\partial}{\partial t} \left( \frac{\partial c}{\partial x} \right) + u_0 \frac{\partial}{\partial x} \left( \frac{\partial c}{\partial x} \right) = 0 \quad (3.15)$$

Using  $cx = \partial c / \partial x$  the equation above may be written as

$$\frac{\partial cx}{\partial t} + u_0 \frac{\partial cx}{\partial x} = 0 \quad (3.16)$$

We note that this form is exactly analogous to that in (3.1) for the concentration itself. Considering (3.6) and employing previous results for the A, B, and D coefficients

$$\begin{aligned} \dot{y}(\alpha) = & \left\{ \left[ 3(x_i - x_{i-1}) (cx_{i-1}^n + cx_i^n) - 6(c_{i-1}^n - c_i^n) \right] \alpha^2 \right. \\ & + \left[ 6(c_{i-1}^n - c_i^n) - 2(2cx_i^n + cx_{i-1}^n)(x_i - x_{i-1}) \right] \alpha \\ & \left. + cx_i^n (x_i - x_{i-1}) \right\} / (x_i - x_{i-1}) \end{aligned} \quad (3.17)$$

Upon rearrangement we obtain

$$\begin{aligned} \dot{y}(\alpha) = & 3\alpha^2 (cx_{i-1}^n + cx_i^n) - \frac{6(c_{i-1}^n - c_i^n)}{(x_i - x_{i-1})} \alpha^2 \\ & + \frac{6(c_{i-1}^n - c_i^n)}{(x_i - x_{i-1})} \alpha - 2(2cx_i^n + cx_{i-1}^n) \alpha + cx_i^n \end{aligned} \quad (3.18)$$

or

$$\begin{aligned} \dot{y}(\alpha) = & \frac{6(\alpha - \alpha^2)}{(x_i - x_{i-1})} c_{i-1}^n + \frac{6(\alpha^2 - \alpha)}{(x_i - x_{i-1})} c_i^n + (3\alpha^2 - 2\alpha) cx_{i-1}^n \\ & + (3\alpha^2 - 4\alpha + 1) cx_i^n \end{aligned} \quad (3.19)$$

Then by analogy

$$cx_i^{n+1} = \dot{y}(\alpha) \quad (3.20)$$

A linear stability analysis is performed to demonstrate the following stability criteria

$$\left| \lambda_2 \right| < \left| \lambda_1 \right| < 1 \quad \text{for } \alpha \leq 1 \quad (3.21)$$

where

$\left| \lambda_1 \right|$  = primary mode

$\left| \lambda_2 \right|$  = a parasitic computational mode sufficiently small relative to unity so that the mode disappears from the solution quite rapidly

In order to perform the computations, initial and boundary conditions for both the concentration and its space derivative must be specified. The specification of the spatial derivative may not be straightforward in practical computations.

The method is extended to the non-uniform velocity case in the following manner. In this case the exact solution to (3.1) requires that the concentration be constant on the trajectory or characteristic curve

$$\frac{dx}{dt} = u(x,t) \quad (3.22)$$

Thus, in the application of (3.14), the interpolation argument corresponds to the point on the x-axis where the trajectory defined by (3.22) crosses it. This point is estimated by means of a suitable integration of  $u(x,t)$  from point  $i$  to  $i-1$  over the time interval  $\tau$ . In order to compute the advection of the concentration derivative, equation (3.16) is written more generally as

$$\frac{\partial cx}{\partial t} + u(x,t) \frac{\partial cx}{\partial x} + cx \frac{\partial u(x,t)}{\partial x} = 0 \quad (3.23)$$



The first two terms are evaluated using the trajectory-estimated  $\alpha$  in the application of (3.20). The contribution of the third term is determined by averaging  $cx$  and  $\partial u/\partial x$  from the point  $i$  to  $i-1$ .

The extension of the technique to two dimensions for the constant velocity case is briefly outlined. However, the treatment for the non-uniform case is not completely apparent. Diffusion may be incorporated within the interpolation scheme but only at the expense of a more severe restriction on the time step than  $\alpha \leq 1$ . By decoupling the diffusion calculations from advection the authors suggest this restriction may be avoided.

#### 4. Method of Second Moments

Egan and Mahoney introduced this scheme in meteorological studies (air pollution transport) [9]. Width correction adjustments were reported by Pedersen and Prahm [10]. Pepper and Baker [11] have developed an elaborate three-dimensional transport algorithm for predicting tritium releases from the Savannah River Nuclear Power Plant.

The basic method involves describing the concentration distribution within each cell of an Eulerian mesh by its first three moments, zeroth (total mass), first (mass center), and second moment (variance). The cell distribution representations are then advected using the velocity components developed from a separate solution scheme. At the end of the time step the resulting individual distributions are combined in a composite and the process is repeated over the subsequent time steps. The scheme is explicit and quasi-Lagrangian. Due to the explicit nature of the advection scheme the particle Courant number must be less than or equal to one to maintain stability.

The method is presented in one-dimension by considering a concentration distribution to be represented by three parameters defined as follows

$$\begin{aligned}
 C_m &= \int_{-0.5}^{+0.5} C(\epsilon_m) d\epsilon \\
 C_m F_m &= \int_{-0.5}^{+0.5} C(\epsilon_m) \epsilon_m d\epsilon \\
 C_m R_m^2 &= 12 \int_{-0.5}^{+0.5} C(\epsilon_m) (\epsilon_m - F_m)^2 d\epsilon
 \end{aligned} \tag{4.1}$$

where

$\epsilon_m \equiv$  relative displacement of material in the mth cell relative to the cell center

$C_m \equiv$  mean (cell) concentration of the distribution

$F_m \equiv$  center of mass of concentration distribution

$R_m^2 \equiv$  scaled second moment of concentration distribution

$R_m^2$  is scaled, multiplied by a factor of 12, such that a rectangular distribution of length  $L$  has  $R_m^2 = L^2$ . In applying the method, rectangular type distributions are maintained in each grid cell. Initially,  $C_m$  is specified and the distribution is assumed to occupy the entire cell. For rectangular type distributions, the integrals in (4.1) above are evaluated by considering for each grid cell the material distribution remaining in the cell and those which entered during the time interval.

Figure 3 illustrates the procedure for advection in one time step

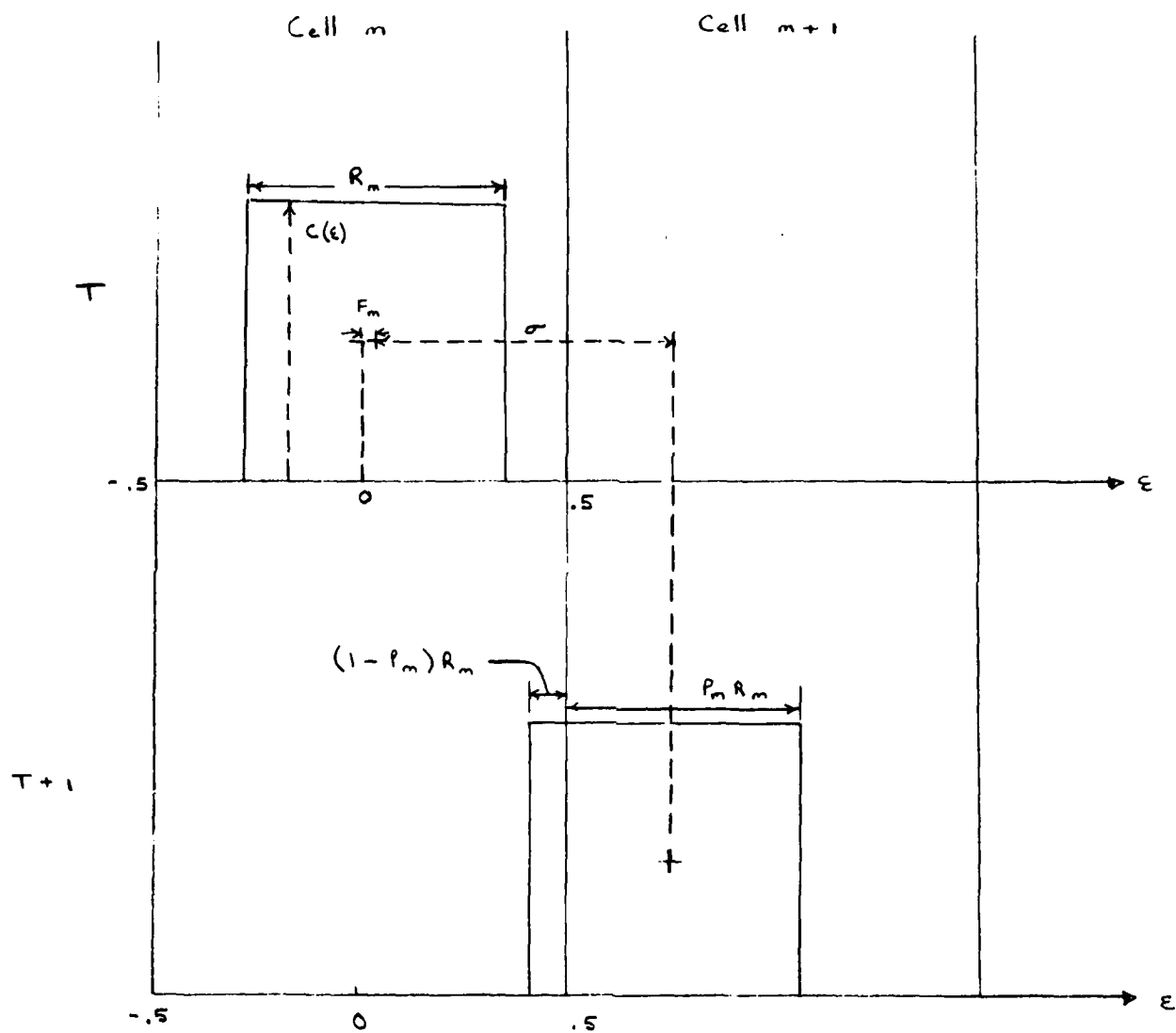


Figure 3. Method of moments advection procedure (one dimension)

of  $\sigma = u\Delta t/\Delta x$ . A proportioning parameter is defined as  $P_m = (F_m + \sigma + R_m/2 - 0.5)/R_m$ . For  $P_m \leq 0$  none of the material is advected into cell  $m+1$ . For  $P_m > 1$  all of the material in cell  $m$  is advected into cell  $m+1$ . For  $0 < P_m < 1$ ,  $P_m C_m$  is advected into cell  $m+1$ , while  $(1 - P_m)C_m$  remains in cell  $m$ . Thus in general, one obtains

$$C_m^{T+1} = C_r + C_a \quad (4.2a)$$

$$C_m^{T+1} F_m^{T+1} = C_r F_r + C_a F_a \quad (4.2b)$$

$$C_m^{T+1} (R^2)_m^{T+1} = C_r \left[ R_r^2 + 12(F_m^{T+1} - F_r)^2 \right] + C_a \left[ R_a^2 + 12(F_m^{T+1} - F_a)^2 \right] \quad (4.2c)$$

where subscripts  $r$  and  $a$  indicate quantities remaining and newly-advected into cell  $m$ , respectively.

$$\text{For } P_m < 0 : C_r = C_m^T, F_r = F_m^T + \sigma, R_r = R_m^T \quad (4.3a)$$

$$P_m > 1 : C_r = 0, F_r = 0, R_r = 0 \quad (4.3b)$$

$$0 < P_m < 1 : C_r = (1 - P_m)C_m^T$$

$$F_r = \frac{(1 - R_m^T + P_m R_m^T)}{2} \quad (4.3c)$$

$$R_r = (1 - P_m)R_m^T$$

$$P_{m-1} < 0 : C_a = 0, F_a = 0, R_a = 0 \quad (4.3d)$$

$$P_{m-1} > 1 : C_a = C_{m-1}^T, F_a = F_{m-1}^T + \sigma - 1,$$

$$R_a = R_{m-1}^T \quad (4.3e)$$

$$\begin{aligned}
0 < P_{m-1} < 1 : C_a &= P_{m-1} C_{m-1}^T \\
F_a &= \frac{(P_{m-1} R_{m-1}^T - 1)}{2} \\
R_a &= P_{m-1} R_{m-1}^T
\end{aligned} \tag{4.3f}$$

A step-shaped distribution will be advected downwind without change of shape. Small diffusive errors will remain when more complicated distributions are advected.

The technique may be extended to two dimensions and, in the following, we employ the notation of Pedersen and Prahm [10]. Two portioning parameters are defined as follows.

$$P_x = \left[ \text{sign}(\sigma_x)(F_x + \sigma_x) - \frac{(1 - R_x)}{2} \right] / R_x \tag{4.4a}$$

$$P_y = \left[ \text{sign}(\sigma_y)(F_y + \sigma_y) - \frac{(1 - R_y)}{2} \right] / R_y \tag{4.4b}$$

These concepts are illustrated in Figure 4. In the most common case,  $0 < P_x < 1$ , and  $0 < P_y < 1$ , and the computational formulae analogous to the one-dimensional case, are given as follows.

Contributions in grid cell (m,n)

$$\begin{aligned}
(C^{T+1})_r &= (1 - P_x)(1 - P_y)C^T \\
(F_x^{T+1})_r &= \frac{(1 - R_x^T + P_x R_x^T)}{2} \text{sign}(\sigma_x) \\
(F_y^{T+1})_r &= \frac{(1 - R_y^T + P_y R_y^T)}{2} \text{sign}(\sigma_y) \\
(R_x^{T+1})_r &= (1 - P_x)R_x^T \\
(R_y^{T+1})_r &= (1 - P_y)R_y^T
\end{aligned} \tag{4.5}$$

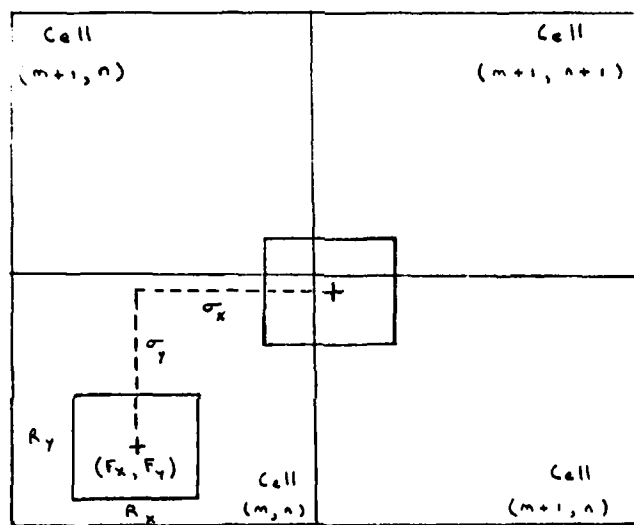


Figure 4. Method of moments advection procedure (two dimensions)

Contributions in cell (m+1 sign ( $\sigma_x$ ), n)

$$\begin{aligned}
 (C)_a^{T+1} &= P_x (1 - P_y) C^T \\
 (F_x)_a^{T+1} &= \frac{(P_x R_x^T - 1)}{2} \text{sign } (\sigma_y) \\
 (F_y)_a^{T+1} &= \frac{(1 - R_y^T + P_y R_y)}{2} \text{sign } (\sigma_y) \\
 (R_x)_a^{T+1} &= P_x R_x^T \\
 (R_y)_a^{T+1} &= (1 - P_y) R_y^T
 \end{aligned} \tag{4.6}$$

Contributions in cell (m, n+1 sign ( $\sigma_y$ ))

$$\begin{aligned}
 (C)_a^{T+1} &= P_y (1 - P_x) C^T \\
 (F_x)_a^{T+1} &= \frac{(1 - R_x^T + P_x R_x)}{2} \text{sign } (\sigma_x) \\
 (F_y)_a^{T+1} &= \frac{(P_y R_y^T - 1)}{2} \text{sign } (\sigma_y) \\
 (R_x)_a^{T+1} &= (1 - P_x) R_x^T \\
 (R_y)_a^{T+1} &= P_y R_y^T
 \end{aligned} \tag{4.7}$$

Contributions in cell  $(m+1 \text{ sign } (\sigma_x), n+1 \text{ sign } (\sigma_y))$

$$\begin{aligned}
 (C)_a^{T+1} &= P_x P_y C^T \\
 (F_x)_a^{T+1} &= \frac{(P_x R_x^T - 1)}{2} \text{sign } (\sigma_x) \\
 (F_y)_a^{T+1} &= \frac{(P_y R_y^T - 1)}{2} \text{sign } (\sigma_y) \\
 (R_x)_a^{T+1} &= P_x R_x^T \\
 (R_y)_a^{T+1} &= P_y R_y^T
 \end{aligned} \tag{4.8}$$

When  $P_x$  and/or  $P_y$  are greater than 1 and/or less than zero, different equations analogous to the one-dimensional case must be applied. We note for an arbitrary cell  $(m,n)$ , 3 distributions may be advected into the cell and 1 may remain. Formulae analogous to (4.2) are employed to compute  $(C)_{m,n}^{T+1}$ ,  $(F_x)_{m,n}^{T+1}$ ,  $(F_y)_{m,n}^{T+1}$ ,  $(R_x)_{m,n}^{T+1}$ , and  $(R_y)_{m,n}^{T+1}$ .

Pedersen and Prahm [10] also limit the width of the distribution such that it must fall within one-cell after the combination process in (4.2) is completed. Analogous limiting may be performed in both coordinates for the two-dimensional case.

This technique may be extended using fractional steps to include the diffusion process as performed by Pepper and Baker [11].

##### 5. Balanced Expansion Technique

Chan [12] has developed a new procedure to construct accurate finite difference advection schemes which are neutrally stable ( $|\lambda| = 1$ ).



By applying the procedure in a systematic manner, the phase error can be reduced. In his development, the following model equation is considered.

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0 \quad (5.1)$$

where

$\phi \equiv$  passive scalar

$x \equiv$  space coordinate

$t \equiv$  time

$u > 0$  and is a constant velocity

A Lagrangian approach is employed by noting that the value of  $\phi$  is preserved along the characteristic  $dx/dt = u$  in  $(x,t)$  space. The general solution is  $\phi(x,t) = F(x - ut)$ , which leads to the following equations in the discretization of (5.1).

$$\begin{aligned} \phi(x, t + \delta t) &= \phi(x - u\delta t, t) \\ \phi(x + u\delta t, t) &= \phi(x, t - \delta t) \end{aligned} \quad (5.2)$$

where

$x = j\delta x$

$t = n\delta t$

$\delta t =$  time increment

$\delta x =$  space increment

The Courant number  $\alpha = u\delta t/\delta x$  is introduced and the procedure is illustrated in Figure 5. The positions of the six quantities  $\phi_{j-1}^{n+1}$ ,  $\phi_{j-1}^n$ ,  $\phi_{j-1}^{n-1}$ ,  $\phi_j^{n+1}$ ,  $\phi_j^n$ ,  $\phi_j^{n-1}$  are symmetric about  $\phi_o$ , which is midway between  $j-1$  and  $j$ . Each of these six quantities is expanded

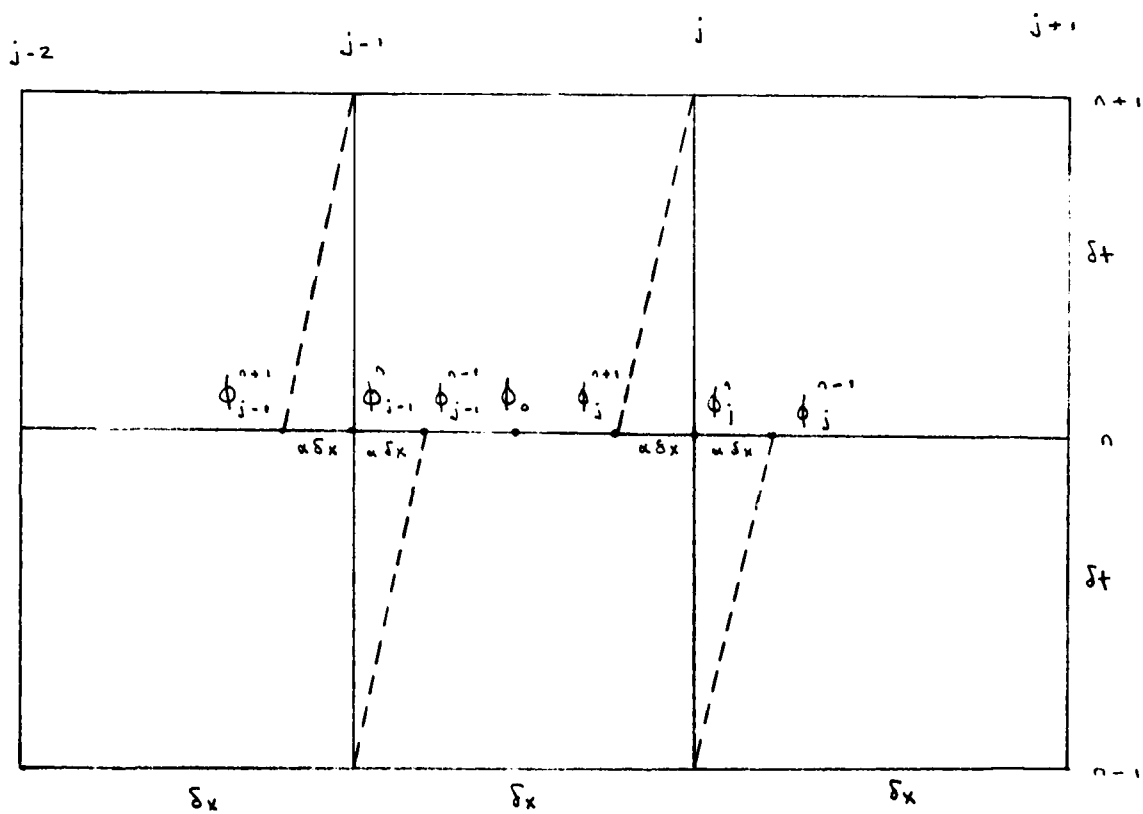


Figure 5. Chan definition of variables

in a Taylor series about  $\phi_0$ . The following balanced differences are constructed. In this manner, all even derivatives in the Taylor's series are eliminated.

$$\begin{aligned}\phi_j^{n-1} - \phi_{j-1}^{n+1} &= 2\left(\alpha + \frac{1}{2}\right) \delta x \phi_x + \frac{2}{3!} \left(\alpha + \frac{1}{2}\right)^3 \delta x^3 \phi_{xxx} \\ &\quad + \frac{2}{5!} \left(\alpha + \frac{1}{2}\right)^5 \delta x^5 \phi^{(5)} + \dots\end{aligned}\tag{5.3}$$

$$\begin{aligned}\phi_j^n - \phi_{j-1}^n &= 2\left(\frac{1}{2}\right) \delta x \phi_x + \frac{2}{3!} \left(\frac{1}{2}\right)^3 \delta x^3 \phi_{xxx} \\ &\quad + \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^{(5)} + \dots\end{aligned}\tag{5.4}$$

$$\begin{aligned}\phi_j^{n+1} - \phi_{j-1}^{n-1} &= 2\left(\frac{1}{2} - \alpha\right) \delta x \phi_x + \frac{2}{3!} \left(\frac{1}{2} - \alpha\right)^3 \delta x^3 \phi_{xxx} \\ &\quad + \frac{2}{5!} \left(\frac{1}{2} - \alpha\right)^5 \delta x^5 \phi^{(5)} + \dots\end{aligned}\tag{5.5}$$

From (5.4) let us solve for  $\delta x \phi_x$ ,

$$\delta x \phi_x = \phi_j^n - \phi_{j-1}^n - \frac{2}{3!} \left(\frac{1}{2}\right)^3 \delta x^3 \phi_{xxx} - \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^{(5)}\tag{5.6}$$

Substituting (5.6) in (5.3) we have

$$\begin{aligned}\phi_j^{n-1} - \phi_{j-1}^{n+1} &= (2\alpha + 1) \left[ \phi_j^n - \phi_{j-1}^n - \frac{2}{3!} \left(\frac{1}{2}\right)^3 \delta x^3 \phi_{xxx} \right. \\ &\quad \left. - \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^{(5)} \right] + \frac{2}{3!} \left(\alpha + \frac{1}{2}\right)^3 \delta x^3 \phi_{xxx} + \frac{2}{5!} \left(\alpha + \frac{1}{2}\right)^5 \delta x^5 \phi^{(5)}\end{aligned}\tag{5.7}$$

Solving for  $\phi_{xxx}$  :

$$\Delta_3 = \frac{2}{3!} \delta x^3 \phi_{xxx} = \frac{\phi_j^{n-1} - \phi_{j-1}^{n+1} - (2\alpha + 1)(\phi_j^n - \phi_{j-1}^n) + \left[ (2\alpha + 1)\left(\frac{1}{2}\right)^5 - \left(\alpha + \frac{1}{2}\right)^5 \right] \frac{2}{5!} \delta x^5 \phi^5}{\left(\alpha + \frac{1}{2}\right)^3 - (2\alpha + 1)\left(\frac{1}{2}\right)^3} \quad (5.8)$$

Substituting (5.8) into (5.6)

$$\begin{aligned} \delta x \phi_x = \phi_j^n - \phi_{j-1}^n - \left(\frac{1}{2}\right)^3 & \left\{ \frac{\phi_j^{n-1} - \phi_{j-1}^{n+1} - (2\alpha + 1)(\phi_j^n - \phi_{j-1}^n) + \left[ (2\alpha + 1)\left(\frac{1}{2}\right)^5 - \left(\alpha + \frac{1}{2}\right)^5 \right] \frac{2}{5!} \delta x^5 \phi^5}{\left(\alpha + \frac{1}{2}\right)^3 - (2\alpha + 1)\left(\frac{1}{2}\right)^3} \right\} \\ & - \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^5 = \phi_j^n - \phi_{j-1}^n - \left(\frac{1}{2}\right)^3 \Delta_3 - \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^5 \end{aligned} \quad (5.9)$$

Using (5.8) and (5.9) in (5.5), we finally obtain

$$\begin{aligned} \phi_j^{n+1} - \phi_{j-1}^{n-1} = 2\left(\frac{1}{2} - \alpha\right) & \left[ \phi_j^n - \phi_{j-1}^n - \left(\frac{1}{2}\right)^3 \Delta_3 - \frac{2}{5!} \left(\frac{1}{2}\right)^5 \delta x^5 \phi^5 \right] \\ & + \left(\frac{1}{2} - \alpha\right)^3 \Delta_3 + \frac{2}{5!} \left(\frac{1}{2} - \alpha\right)^5 \delta x^5 \phi^5 \end{aligned} \quad (5.10a)$$

$$\begin{aligned} \phi_j^{n+1} - \phi_j^{n-1} = (1 - 2\alpha) & \left( \phi_j^n - \phi_{j-1}^n \right) + \left[ \left(\frac{1}{2} - \alpha\right)^3 - (1 - 2\alpha)\left(\frac{1}{2}\right)^3 \right] \Delta_3 \\ & + \frac{2}{5!} \delta x^5 \phi^5 \left[ \left(\frac{1}{2} - \alpha\right)^5 - (1 - 2\alpha)\left(\frac{1}{2}\right)^5 \right] \end{aligned} \quad (5.10b)$$

From auxiliary relations developed in Table II, we simplify the above

$$\begin{aligned} \phi_j^{n+1} - \phi_j^{n-1} = (1 - 2\alpha) & \left( \phi_j^n - \phi_{j-1}^n \right) - \frac{\alpha}{2} (2\alpha - 1)(\alpha - 1) \\ & \times \left\{ \frac{\phi_j^{n-1} - \phi_{j-1}^{n+1} - (2\alpha + 1)(\phi_j^n - \phi_{j-1}^n) + \left[ (2\alpha + 1)\left(\frac{1}{2}\right)^5 - \left(\alpha + \frac{1}{2}\right)^5 \right] \frac{2}{5!} \delta x^5 \phi^5}{\frac{\alpha}{2} (2\alpha + 1)(\alpha + 1)} \right\} \\ & + \frac{2}{5!} \delta x^5 \phi^5 \left[ \left(\frac{1}{2} - \alpha\right)^5 - (1 - 2\alpha)\left(\frac{1}{2}\right)^5 \right] \end{aligned} \quad (5.11)$$

Table II. Chan Auxillary Relations

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$$\left(\alpha + \frac{1}{2}\right)^3 - (2\alpha + 1)\left(\frac{1}{2}\right)^3 = \frac{\alpha}{2} (2\alpha + 1)(\alpha + 1)$$

$$\left(\frac{1}{2} - \alpha\right)^3 - (1 - 2\alpha)\left(\frac{1}{2}\right)^3 = -\frac{\alpha}{2} (2\alpha - 1)(\alpha - 1)$$

$$\left(\alpha + \frac{1}{2}\right)^4 - \left(\frac{1}{2}\right)^4 = \alpha\left(\alpha^3 + 2\alpha^2 + \frac{3}{2}\alpha + \frac{1}{2}\right)$$

$$\left(\frac{1}{2} - \alpha\right)^4 - \left(\frac{1}{2}\right)^4 = \alpha\left(\alpha^3 - 2\alpha^2 + \frac{3}{2}\alpha - \frac{1}{2}\right)$$


---

$$\begin{aligned}\phi_j^{n+1} &= \phi_j^{n-1} + \frac{(1-2\alpha)(1-\alpha)}{(1+2\alpha)(1+\alpha)} (\phi_{j-1}^{n+1} - \phi_j^{n-1}) \\ &\quad + \frac{(\alpha+1)(1-2\alpha) + (2\alpha-1)(\alpha-1)}{(\alpha+1)} (\phi_j^n - \phi_{j-1}^n) \end{aligned} \quad (5.12)$$

$$\begin{aligned} &- \left\{ \frac{(2\alpha-1)(\alpha-1)}{(2\alpha+1)(\alpha+1)} \left[ (2\alpha+1)\left(\frac{1}{2}\right)^5 - \left(\alpha + \frac{1}{2}\right)^5 \right] \right. \\ &\quad \left. + \left[ -\left(\frac{1}{2} - \alpha\right)^5 + (1-2\alpha)\left(\frac{1}{2}\right)^5 \right] \right\} \frac{2}{5!} \delta x^5 \phi^5 \end{aligned}$$

We continue to simplify by noting

$$\begin{aligned} (\alpha+1)(1-2\alpha) + (2\alpha-1)(\alpha-1) &= -2\alpha^2 - \alpha + 1 + 2\alpha^2 - 3\alpha + 1 \\ &= -4\alpha + 2 = 2(1-2\alpha) \end{aligned}$$

and the  $\delta x^5 \phi^5$  term may be written as

$$\begin{aligned} &\left\{ \frac{(2\alpha-1)(\alpha-1)}{(\alpha+1)} \left[ \left(\frac{1}{2}\right)^4 - \left(\alpha + \frac{1}{2}\right)^4 \right] + (1-2\alpha) \left[ \left(\frac{1}{2}\right)^4 - \left(\frac{1}{2} - \alpha\right)^4 \right] \right\} \frac{\delta x^5 \phi^5}{5!} \\ &= \left\{ \frac{(2\alpha-1)(\alpha-1)}{(\alpha+1)} \left[ \left(\frac{1}{2}\right)^4 - \left(\alpha + \frac{1}{2}\right)^4 \right] + (1-2\alpha)(\alpha+1) \left[ \left(\frac{1}{2}\right)^4 - \left(\frac{1}{2} - \alpha\right)^4 \right] \right\} \frac{\delta x^5 \phi^5}{5!} = f \phi^5 \end{aligned} \quad (5.13)$$

Thus

$$\begin{aligned}\phi_j^{n+1} &= \phi_j^{n-1} + \frac{(1-2\alpha)(1-\alpha)}{(1+2\alpha)(1+\alpha)} (\phi_{j-1}^{n+1} - \phi_j^{n-1}) \\ &\quad + \frac{2(1-2\alpha)}{(\alpha+1)} (\phi_j^n - \phi_{j-1}^n) + f \phi^5 \end{aligned} \quad (5.14)$$

Dropping the truncation error a discrete formula for calculating  $\phi_j^{n+1}$  is developed without attempting to evaluate derivatives. The computational scheme in (5.14) is a three time level scheme containing information at only two space points ( $j$  and  $j-1$ ). The scheme is explicit if computations are performed sequentially in the downstream direction.

Chan obtains several other formulae by using balanced pairs (centered about  $\phi_0$ ). In all cases, stability is governed by  $0 \leq \alpha \leq 1$ . By including more points symmetric about  $\phi_0$ , it is possible to develop formulae which successively eliminate higher order odd space derivatives. In (5.14)  $\phi_x$  and  $\phi_{xxx}$  have been eliminated. Chan presents schemes which eliminate  $\phi^5$  as well, along with two additional formulae in which  $\phi_{xxx}$  is eliminated. The essential characteristics of the balanced expansion scheme are: (1) all even space derivatives are eliminated, which Chan notes is sufficient to insure  $|\lambda| = 1$ , and (2) successive elimination of higher order space derivatives reduces the phase error.

Chan modifies (5.14) for the case of diffusion; namely,

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = v \frac{\partial^2 \phi}{\partial x^2} \quad (5.15)$$

where  $v$  is a diffusion coefficient. Figure 6 is employed in developing the method. Unlike in Figure 5,  $\phi_j^{n+1}$  is not equal to  $\tilde{\phi}_j^{n+1}$ , which is the value of  $\phi$  located at  $\alpha \delta x$  to the left of  $\phi_j^n$ . He notes that the fluid particle originally at  $\tilde{\phi}_j^{n+1}$  does move to position  $\phi_j^{n+1}$  at the end of the  $\delta t$  increment; however, the diffusion process has changed the  $\phi$  value associated with the particle. Using a forward-time, central space, finite difference scheme for  $D\phi/Dt = v \partial^2 \phi / \partial x^2$ ,

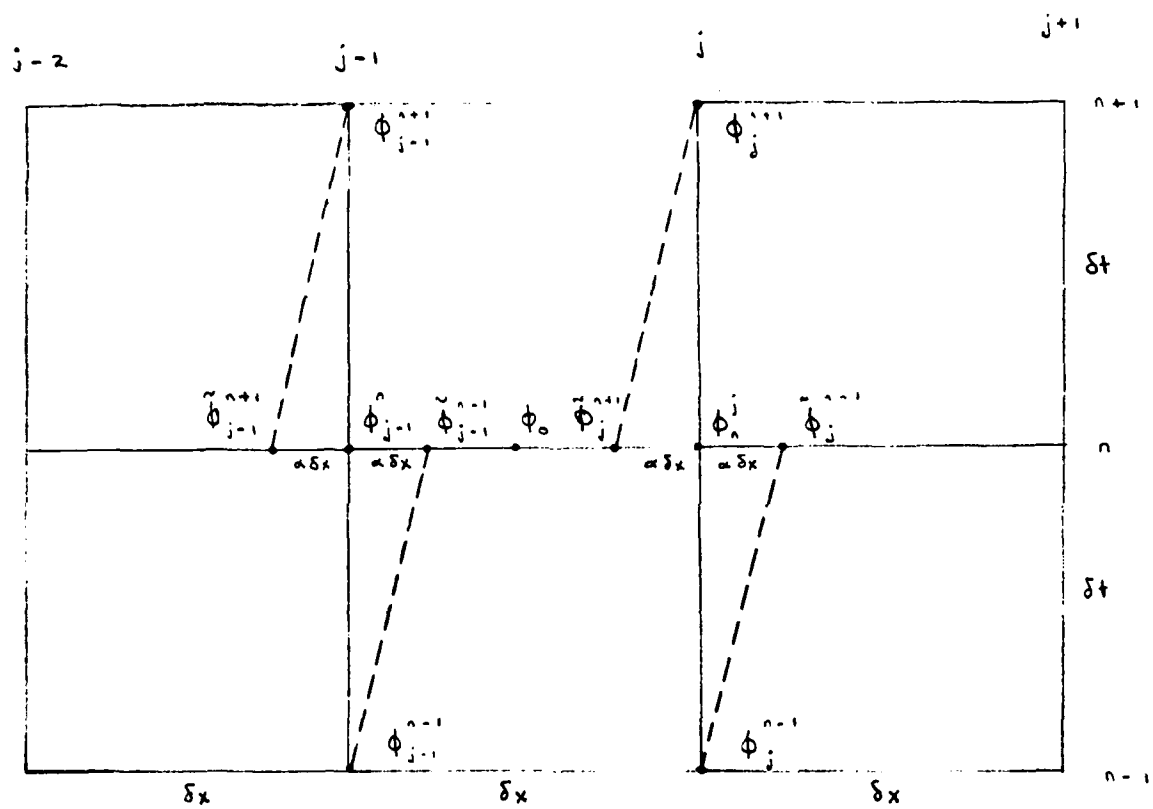


Figure 6. Chan definition for extension to include diffusion



$D/Dt$  is the Lagrangian derivative, Chan obtains

$$\phi_j^{n+1} = \tilde{\phi}_j^{n+1} + \beta(\phi_{j+1}^{n+1} - 2\tilde{\phi}_j^{n+1} + \phi_{j-1}^{n+1}) \quad (5.16)$$

where  $\beta = v\delta t/\delta x$ . For stability  $0 \leq \beta \leq 1/2$ . Similarly, because of diffusion,  $\phi_j^{n-1}$  is not equal to  $\tilde{\phi}_j^{n+1}$ . They are related by

$$\tilde{\phi}_j^{n-1} = \phi_j^{n-1} + \beta(\phi_{j+1}^{n-1} - 2\phi_j^{n-1} + \phi_{j-1}^{n-1}) \quad (5.17)$$

In analogy, with the original development for advection only, the six quantities  $\tilde{\phi}_{j-1}^{n+1}$ ,  $\phi_{j-1}^n$ ,  $\tilde{\phi}_{j-1}^{n-1}$ ,  $\tilde{\phi}_j^{n+1}$ ,  $\phi_j^n$ , and  $\tilde{\phi}_j^{n-1}$  are expanded in Taylor series about  $\phi_0$  to give

$$\begin{aligned} \tilde{\phi}_j^{n+1} = \tilde{\phi}_{j-1}^{n-1} + \frac{(1-2\alpha)(1-\alpha)}{(1+2\alpha)(1+\alpha)} (\tilde{\phi}_{j-1}^{n+1} - \tilde{\phi}_j^{n-1}) \\ + \frac{2(1-2\alpha)}{(\alpha+1)} (\phi_j^n - \phi_{j-1}^n) \end{aligned} \quad (5.18)$$

The solution procedure consists then of the following three steps

1. Compute  $\tilde{\phi}_j^{n-1}$  using (5.17) for the entire space domain
2. Use (5.18) to compute  $\tilde{\phi}_j^{n+1}$  over the space domain
3. Use (5.16) to compute  $\phi_j^{n+1}$

The techniques presented and preliminary testing by Chan show that the advection-diffusion schemes are very accurate. Unfortunately only the one dimensional case is considered with constant coefficients. Extensions to multi-dimensional problems, flows with non-uniform

velocity and diffusion, and mesh with variable spacings have not been reported.

#### 6. Stone and Brian Technique [13]

In their development, the usual one-dimensional equation is considered

$$D \frac{\partial^2 u}{\partial x^2} - V \frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} = 0 \quad (6.1)$$

where

$D \equiv$  diffusion coefficient (assumed constant)

$V \equiv$  constant velocity

$u \equiv$  concentration of a given material

Since  $u(x,t) = \sum_{w=1}^{\infty} A_w e^{-w^2 \pi^2 D t} \sin w \pi (x - Vt)$  satisfies (6.1), it constitutes a solution for the appropriate boundary conditions.

A general form of finite difference approximations to (6.1) is considered as follows

$$-D L_x^2(u) + V L_x(u) + L_t(u) = 0 \quad (6.2)$$

where

$L_x^2(u) \equiv$  approximation to  $\partial^2 u / \partial x^2$

$L_x(u) \equiv$  approximation to  $\partial u / \partial x$

$L_t(u) \equiv$  approximation to  $\partial u / \partial t$

Stone and Brian note, that the corresponding finite difference solution to (6.2) with the corresponding boundary conditions may be written as

$$u_{j,n} = \sum_{w=1}^{J-1} A_w p^n \sin w\pi (j\Delta x - V\phi n\Delta t) \quad (6.3)$$

in which  $p$  and  $\phi$  depend upon  $w\pi\Delta x$ ,  $V\Delta t/\Delta x$ , and  $D\Delta t/\Delta x^2$ , and on the finite difference approximation employed and  $J$  represents the number segments into which  $x$  is divided.

It is their objective to evaluate the accuracy of various finite-difference approximations to (6.1) by comparing  $V$  with  $\phi V$  and  $e^{-w^2\pi^2 D\Delta t}$  with  $p$ . For a perfect equation  $\phi = 1$  for all  $J-1$  frequencies. In the special case,  $D = 0$ ,  $p = 1$ ; however, for  $D \geq 0$ ,  $p$  would be smaller for high-frequency harmonics than for low frequency harmonics.

The general finite difference analog to (6.1) is written as follows.

$$\begin{aligned} -D \left[ \Delta x^2 \frac{(u_{j,n} + u_{j,n+1})}{2} \right] + \frac{V}{\Delta x} \left[ a(u_{j+1,n} - u_{j,n}) \right. \\ \left. + \frac{\epsilon}{2} (u_{j,n} - u_{j-1,n}) + c(u_{j+1,n+1} - u_{j,n+1}) \right. \\ \left. + d(u_{j,n+1} - u_{j-1,n+1}) \right] + \frac{1}{\Delta t} \left[ g(u_{j,n+1} - u_{j,n}) \right. \\ \left. + \frac{\theta}{2} (u_{j-1,n+1} - u_{j-1,n}) + m(u_{j+1,n+1} - u_{j+1,n}) \right] = 0 \end{aligned} \quad (6.4)$$

where

$$a + \frac{\epsilon}{2} + c + d = 1$$

$$g + \frac{\theta}{2} + m = 1$$

$$\Delta x^2 u_{j,n} = (u_{j+1,n} - 2u_{j,n} + u_{j-1,n})/\Delta x^2$$

A Crank-Nicolson approximation is employed for the diffusion term, and the approximations for  $\partial u/\partial x$  and  $\partial u/\partial t$  involve the same six points.

If one considers  $u_{j,n} = \eta^n e^{i w \pi j \Delta x}$  and substitutes this relation in (6.4), one obtains a relation for  $\eta = p e^{-i w \pi V \phi \Delta t}$  wherein,

$$p^2 = \frac{\left\{ g + \beta \left( a - \frac{\epsilon}{2} \right) + \left[ \left( \frac{\theta}{2} + m \right) - \beta \left( a - \frac{\epsilon}{2} \right) \right] \cos w \pi \Delta x - \alpha \sin^2 \left( \frac{w \pi \Delta x}{2} \right) \right\}^2 + \left\{ \left[ \beta \left( a + \frac{\epsilon}{2} \right) + \left( \frac{\theta}{2} - m \right) \right] \sin (w \pi \Delta x) \right\}^2}{\left\{ g + \beta (d - c) + \left[ \left( \frac{\theta}{2} + m \right) - \beta (d - c) \right] \cos w \pi \Delta x + \alpha \sin^2 \left( \frac{w \pi \Delta x}{2} \right) \right\}^2 + \left\{ \left[ \beta (c + d) - \left( \frac{\theta}{2} - m \right) \right] \sin (w \pi \Delta x) \right\}^2} \quad (6.5)$$

and

$$\phi = \frac{1}{\beta w \pi \Delta x} \left\{ \tan^{-1} \frac{\left[ \beta \left( a + \frac{\epsilon}{2} \right) + \left( \frac{\theta}{2} - m \right) \right] \sin w \pi \Delta x}{g + \beta \left( a - \frac{\epsilon}{2} \right) + \left[ \left( \frac{\theta}{2} + m \right) - \beta \left( a - \frac{\epsilon}{2} \right) \right] \cos w \pi \Delta x - \alpha \sin^2 \left( \frac{w \pi \Delta x}{2} \right)} + \tan^{-1} \frac{\beta (c + d) - \left( \frac{\theta}{2} - m \right) \sin w \pi \Delta x}{g + \beta (d - c) + \left[ \left( \frac{\theta}{2} + m \right) - \beta (d - c) \right] \cos w \pi \Delta x + \alpha \sin^2 \left( \frac{w \pi \Delta x}{2} \right)} \right\} \quad (6.6)$$

where

$$\beta = \frac{V \Delta t}{\Delta x}$$

$$\alpha = \frac{2 D \Delta t}{\Delta x^2}$$

From (6.5) in order for  $p = 1$  for  $D = 0 \rightarrow \alpha = 0$ , we must have

$$d - c = a - \epsilon/2 \quad \text{and} \quad c + d = a + \epsilon/2 \rightarrow a = d, \quad c = \epsilon/2 \quad \text{and}$$

$-\theta/2 + m = \theta/2 - m \rightarrow m = \theta/2$ . Considering the previous restrictions on these coefficients we obtain

$$a + \frac{\epsilon}{2} + c + d = 1 = 2a + \epsilon \quad (6.7)$$

$$g + \frac{\theta}{2} + m = 1 = g + \theta$$

Considering the above relations, and  $D = 0$ , we now evaluate (6.6)

$$\phi = \frac{1}{\beta w \pi \Delta x} \left\{ \tan^{-1} \frac{\frac{\beta}{2} \sin w \pi \Delta x}{(1 - \theta) + \beta \left( \frac{1}{2} - \epsilon \right) + \left[ \theta - \beta \left( \frac{1}{2} - \epsilon \right) \right] \cos w \pi \Delta x} \right. \\ \left. + \tan^{-1} \frac{\frac{\beta}{2} \sin w \pi \Delta x}{(1 - \theta) + \beta \left( \frac{1}{2} - \epsilon \right) + \left[ \theta - \beta \left( \frac{1}{2} - \epsilon \right) \right] \cos w \pi \Delta x} \right\} \quad (6.8a)$$

$$\phi = \frac{2}{\beta w \pi \Delta x} \left\{ \tan^{-1} \frac{\frac{\beta}{2} \sin w \pi \Delta x}{1 + \left[ \beta \left( \frac{1}{2} - \epsilon \right) - \theta \right] (1 - \cos w \pi \Delta x)} \right\} \quad (6.8b)$$

If one takes the limit of (6.8b) as  $\beta \rightarrow 0$ , noting  $\tan^{-1} x \approx x$ , as  $x \rightarrow 0$

$$\lim_{\beta \rightarrow 0} \phi = \frac{\frac{\sin(w \pi \Delta x)}{(w \pi \Delta x)}}{1 - \theta [1 - \cos(w \pi \Delta x)]} \\ = \frac{1 - \frac{(w \pi \Delta x)^2}{3!} + \frac{(w \pi \Delta x)^4}{5!} - \frac{(w \pi \Delta x)^6}{7!}}{1 - \theta \left[ \frac{(w \pi \Delta x)^2}{2!} - \frac{(w \pi \Delta x)^4}{4!} + \frac{(w \pi \Delta x)^6}{6!} \dots \right]} \quad (6.9)$$

If  $\theta = 1/3$ , we match terms through the second order and  $\lim_{\beta \rightarrow 0} \phi \approx 1$ .

Stone and Brian note that  $\epsilon = 1/2$  is the best value for the single

remaining degree of freedom. They note  $\lim_{\beta \rightarrow 0} \frac{\partial \phi}{\partial \beta} = 0$  for  $\epsilon = 1/2$ ,

$\theta = 1/3$  . Thus  $\theta = 1/3$  insures good values of  $\phi$  for the low frequency harmonics ( $w\pi$  small) as  $\beta \rightarrow 0$  , and  $\epsilon = 1/2$  insures that these values of  $\phi$  do not change rapidly for a range of  $\beta$  slightly greater than zero.

Collecting all previous results ( $\epsilon = 1/2$  ,  $\theta = 1/3$  ,  $a = 1/4$  ,  $d = 1/4$  ,  $c = 1/4$  ,  $m = 1/6$  ,  $g = 2/3$ ) we obtain rewriting (6.4) the following scheme.

$$\begin{aligned}
 & -D \left[ \Delta x^2 \frac{(u_{j,n} + u_{j,n+1})}{2} \right] + \frac{V}{\Delta x} \left[ \frac{1}{4} (u_{j+1,n} - u_{j,n}) \right. \\
 & + \frac{1}{4} (u_{j,n} - u_{j-1,n}) + \frac{1}{4} (u_{j+1,n+1} - u_{j,n+1}) \\
 & \left. + \frac{1}{4} (u_{j,n+1} - u_{j-1,n+1}) \right] + \frac{1}{\Delta t} \left[ \frac{2}{3} (u_{j,n+1} - u_{j,n}) \right. \\
 & \left. + \frac{1}{6} (u_{j-1,n+1} - u_{j-1,n}) + \frac{1}{6} (u_{j+1,n+1} - u_{j+1,n}) \right] = 0
 \end{aligned} \tag{6.10}$$

The interesting feature in (6.10) is the spatial time derivative or "spread" time derivative. If we also return to (6.5), we now obtain for the scheme in (6.10)

$$p^2 = \frac{\left[ \frac{2}{3} + \frac{1}{3} \cos w\pi\Delta x - \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 + \left[ \frac{\beta}{2} \sin (w\pi\Delta x) \right]^2}{\left[ \frac{2}{3} + \frac{1}{3} \cos w\pi\Delta x + \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 + \left[ \frac{\beta}{2} \sin (w\pi\Delta x) \right]^2} \leq 1 \tag{6.11}$$

for all  $w\pi\Delta x$  and for all  $\alpha$  and  $\beta$  . Therefore the method is unconditionally stable with no time step restriction. Stone and Brian also

consider a scheme with  $\epsilon = 2/3$ ,  $\theta = 1/3$ ,  $a = 1/6 = d$ ,  $g = 2/3$ ,  
 $c = 1/3$ ,  $m = 1/6$ ; then one obtains

$$\begin{aligned}
 & -D \left[ \Delta x^2 \frac{(u_{j,n} + u_{j,n+1})}{2} \right] + \frac{v}{\Delta x} \left[ \frac{1}{6} (u_{j+1,n} - u_{j,n}) \right. \\
 & + \frac{1}{3} (u_{j,n} - u_{j-1,n}) + \frac{1}{3} (u_{j+1,n+1} - u_{j,n+1}) \\
 & + \frac{1}{6} (u_{j,n+1} - u_{j-1,n+1}) \left. \right] + \frac{1}{\Delta t} \left[ \frac{2}{3} (u_{j,n+1} - u_{j,n}) \right. \\
 & \left. + \frac{1}{6} (u_{j-1,n+1} - u_{j-1,n}) + \frac{1}{6} (u_{j+1,n+1} - u_{j+1,n}) \right] = 0
 \end{aligned} \tag{6.12}$$

If we evaluate (6.5) for this scheme, we obtain

$$\begin{aligned}
 & \left[ \frac{2}{3} + \beta \left( -\frac{1}{6} \right) + \left( \frac{1}{3} + \frac{\beta}{6} \right) \cos w\pi\Delta x - \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 \\
 & + \left[ \frac{\beta}{2} \sin (w\pi\Delta x) \right]^2 \\
 p^2 = & \frac{\left[ \frac{2}{3} + \beta \left( -\frac{1}{6} \right) + \left( \frac{1}{3} + \frac{\beta}{6} \right) \cos w\pi\Delta x + \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2}{\left[ \frac{2}{3} + \beta \left( -\frac{1}{6} \right) + \left( \frac{1}{3} + \frac{\beta}{6} \right) \cos w\pi\Delta x - \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2} + \frac{\left[ \frac{\beta}{2} \sin (w\pi\Delta x) \right]^2}{\left[ \frac{1}{2} + \frac{1}{2} \cos (w\pi\Delta x) + \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 + \left[ \frac{1}{2} \sin (w\pi\Delta x) \right]^2}
 \end{aligned} \tag{6.13}$$

Letting  $\beta = 1$ ,

$$p^2 = \frac{\left[ \frac{1}{2} + \frac{1}{2} \cos (w\pi\Delta x) - \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 + \left[ \frac{1}{2} \sin (w\pi\Delta x) \right]^2}{\left[ \frac{1}{2} + \frac{1}{2} \cos (w\pi\Delta x) + \alpha \sin^2 \left( \frac{w\pi\Delta x}{2} \right) \right]^2 + \left[ \frac{1}{2} \sin (w\pi\Delta x) \right]^2}$$

From the above, if  $\beta > 1$ , the scheme will become unstable. For this

reason, the scheme is not further considered.

Stone and Brian consider the use of a cyclic set of difference equations. If  $N$  different finite-difference equations are used over  $N$  time steps and the cycle repeated, then in (6.3)

$$p = (p_I p_{II} \dots p_N)^{1/N}$$

$$\phi = \frac{\phi_I + \phi_{II} + \dots + \phi_N}{N} \quad (6.14)$$

Stone and Brian considered  $N = 3$  and developed a different  $\theta$  for  $\epsilon = 1/2$  in each of three finite difference schemes. In each scheme  $p = 1$  for  $D = 0$  and the previous relationships among the coefficients are sufficient to completely define the scheme once  $\theta$  is determined. Consider (6.9) as follows:

$$\lim_{\beta \rightarrow 0} \phi = \frac{\left[ \lim_{\beta \rightarrow 0} (\phi_I) + \lim_{\beta \rightarrow 0} (\phi_{II}) + \lim_{\beta \rightarrow 0} (\phi_{III}) \right]}{3} = 1 \quad (6.15)$$

Letting

$$ND = -\frac{(w\pi\Delta x)^2}{3!} + \frac{(w\pi\Delta x)^4}{5!} - \frac{(w\pi\Delta x)^6}{7!}$$

and

$$DD = \frac{(w\pi\Delta x)^2}{2!} - \frac{(w\pi\Delta x)^4}{4!} + \frac{(w\pi\Delta x)^6}{6!}$$

$$\left( \frac{1 + ND}{1 - \theta_1 DD} + \frac{1 + ND}{1 - \theta_2 DD} + \frac{1 + ND}{1 - \theta_3 DD} \right) = 3 \quad (6.16)$$



Equating the first three powers in  $(w\pi\Delta x)$  three simultaneous equations are obtained in terms of  $\theta_1$ ,  $\theta_2$ , and  $\theta_3$ . This cyclic use of three different difference equations is shown to be superior to the multiple application of the single equation considered previously.

## 7. An Analysis of the Numerical

### Solution of the Transport Equation

Gray and Pinder [14] consider the one-dimensional transport equation with constant velocity, written in their notation as

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \quad (7.1)$$

where

$c \equiv$  constituent concentration

$u \equiv$  transport velocity

$x \equiv$  space coordinate

$t \equiv$  time coordinate

$D \equiv$  diffusion coefficient (constant)

As in previous work, the general solution to (7.1) is considered as a Fourier series.

$$c = \sum_{n=-\infty}^{\infty} c_n \exp(i\beta_n t + i\sigma_n x), \text{ where } |x - ut| \leq 1 \quad (7.2)$$

and  $\beta_n$  is the (time) frequency of the  $n$ th component,  $\sigma_n$  is the spatial frequency, and  $i = \sqrt{-1}$ . If one considers a single component in (7.2) and substitutes it into (7.1), the following relationship is obtained

$$\beta_n + u\sigma_n - iD\sigma_n^2 = 0 \quad (7.3)$$

$$\beta_n = \sigma_n (iD\sigma_n - u) \quad (7.4)$$

Thus for a single component solution, one obtains

$$c \sim c_n \exp [i\sigma_n(x - ut)] \exp \left( -D\sigma_n^2 t \right) \quad (7.5)$$

where the first exponential describes the translation and the second describes the amplitude modulation of a Fourier component with time.

From (7.2) for a single component

$$c_{t+\Delta t} = c_n \exp [i\beta_n(t + \Delta t)] \exp (i\sigma_n x) \quad (7.6)$$

$$= c_n \exp (i\beta_n t + i\sigma_n x) \exp (i\beta_n \Delta t) = c_t \exp (i\beta_n \Delta t)$$

Thus  $\exp (i\beta_n \Delta t)$  is considered an eigenvalue,  $\lambda_n$ .

Let the eigenvalue of the nth Fourier component obtained from the numerical scheme be denoted by  $\lambda'_n$ . Considering the computed and analytical components after a time such that the analytical wave has propagated one wavelength, the number of time steps required is given as follows.

$$N_n = \frac{L_n}{u\Delta t} = \frac{L_n}{\Delta x} \frac{\Delta x}{u\Delta t} \quad (7.7)$$

where  $L_n$  is the wavelength of the nth component. The ratio of the computed to actual amplitude after one wavelength is given by

$$\left[ \frac{|\lambda'_n|}{|\exp(i\beta_n \Delta t)|} \right]^{N_n} = \left[ \frac{|\lambda'_n|}{\exp(-\sigma_n^2 D \Delta t)} \right]^{N_n} = \left[ \frac{|\lambda'_n|}{\exp(-4\pi^2 D' \left[ \left( \frac{\Delta x}{L_n} \right)^2 \right])} \right]^{L_n / \Delta x v} \quad (7.8)$$

where

$$v = \frac{u \Delta t}{\Delta x}$$

$$D' = \frac{D \Delta t}{\Delta x^2}$$

The phase lag  $\theta_n$  after one complete wavelength is defined as

$$\theta_n = \theta'_n N_n - 2\pi \quad \text{with} \quad e^{i\theta'_n} = \frac{\lambda'_n}{|\lambda'_n|} \quad (7.9)$$

Equations (7.8) and (7.9) provide the mechanism for evaluation of alternate schemes for (7.1). Gray and Pinder present a finite element scheme using chapeau basis functions as follows

$$\begin{aligned} & \frac{1}{6} \left[ \frac{c_{i+1,k+1} - c_{i+1,k}}{\Delta t} + 4 \left( \frac{c_{i,k+1} - c_{i,k}}{\Delta t} \right) + \frac{c_{i-1,k+1} - c_{i-1,k}}{\Delta t} \right] \\ & + u \left[ \epsilon \frac{c_{i+1,k+1} - c_{i-1,k+1}}{2\Delta x} + (1 - \epsilon) \frac{c_{i+1,k} - c_{i-1,k}}{2\Delta x} \right] \\ & - D \left[ \epsilon \frac{c_{i+1,k+1} - 2c_{i,k+1} + c_{i-1,k+1}}{\Delta x^2} \right. \\ & \left. + (1 - \epsilon) \frac{c_{i+1,k} - 2c_{i,k} + c_{i-1,k}}{\Delta x^2} \right] \end{aligned} \quad (7.10)$$

If we rewrite (7.10) in operator notation with

$$\delta x = c_{i+1} - c_{i-1} \quad \mu x = \frac{c_{i+1} + c_{i-1}}{2}$$

we obtain the following compact relation.

$$\left( \frac{2}{3} + \frac{ux}{3} + \frac{u\Delta t}{\Delta x} \epsilon \frac{\delta x}{2} - \frac{D\Delta t}{\Delta x^2} \epsilon \delta x^2 \right) c^{k+1} \quad (7.11)$$

$$= \left[ \frac{2}{3} + \frac{ux}{3} - \frac{u\Delta t}{\Delta x} (1 - \epsilon) \frac{\delta x}{2} + \frac{D\Delta t}{\Delta x^2} (1 - \epsilon) \delta x^2 \right] c^k$$

If we consider  $c_{i+1}^k = c_{i+1,k} = e^{\alpha k \Delta t} e^{i \sigma_n \Delta x}$  for the  $n$ th Fourier component and substitute into (7.11) and note for  $\theta = \sigma_n \Delta x$

$$\sin^2 \theta = \frac{1 - \cos 2\theta}{2} = \frac{e^{i2\theta} + e^{-i2\theta} - 2}{-4}$$

$$i \sin \theta = \frac{e^{i\theta} - e^{-i\theta}}{2} \quad \cos \theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

we may write directly the relation for  $\lambda'_n$ .

$$\lambda'_n = \frac{c^{k+1}}{c^k} = \frac{\frac{2}{3} + \frac{\cos \sigma_n \Delta x}{3} - (1 - \epsilon) [v i \sin \sigma_n \Delta x + 2D(1 - \cos \sigma_n \Delta x)]}{\frac{2}{3} + \frac{\cos \sigma_n \Delta x}{3} + \epsilon [v i \sin \sigma_n \Delta x + 2D(1 - \cos \sigma_n \Delta x)]} \quad (7.12)$$

For stability  $|\lambda'_n| \leq 1$ , which requires  $1 \geq \epsilon \geq 0.5$ .

In their paper, Gray and Pinder consider the following finite difference approximation to (7.1) written in compressed operator notation.

$$\left( 1 + \frac{u\Delta t}{\Delta x} \epsilon \frac{\delta x}{2} - \frac{D\Delta t}{\Delta x^2} \epsilon \delta x^2 \right) c^{k+1} \quad (7.13)$$

$$= \left[ 1 - \frac{u\Delta t}{\Delta x} (1 - \epsilon) \frac{\delta x}{2} + \frac{D\Delta t}{\Delta x^2} (1 - \epsilon) \delta x^2 \right] c^k$$

The essential difference between (7.11) and (7.13) is embodied in the treatment of  $\partial c / \partial t$ . In (7.11) a spatial weighted "spread" time derivative approach is employed, while in (7.13) the time derivative is not spatially weighted.

The corresponding eigenvalue for (7.13) is written below as follows

$$\lambda'_n = \frac{c^{k+1}}{c^k} = \frac{1 - (1 - \epsilon)[v_i \sin \sigma_n \Delta x + 2D'(1 - \cos \sigma_n \Delta x)]}{1 + \epsilon[v_i \sin \sigma_n \Delta x + 2D'(1 - \cos \sigma_n \Delta x)]} \quad (7.14)$$

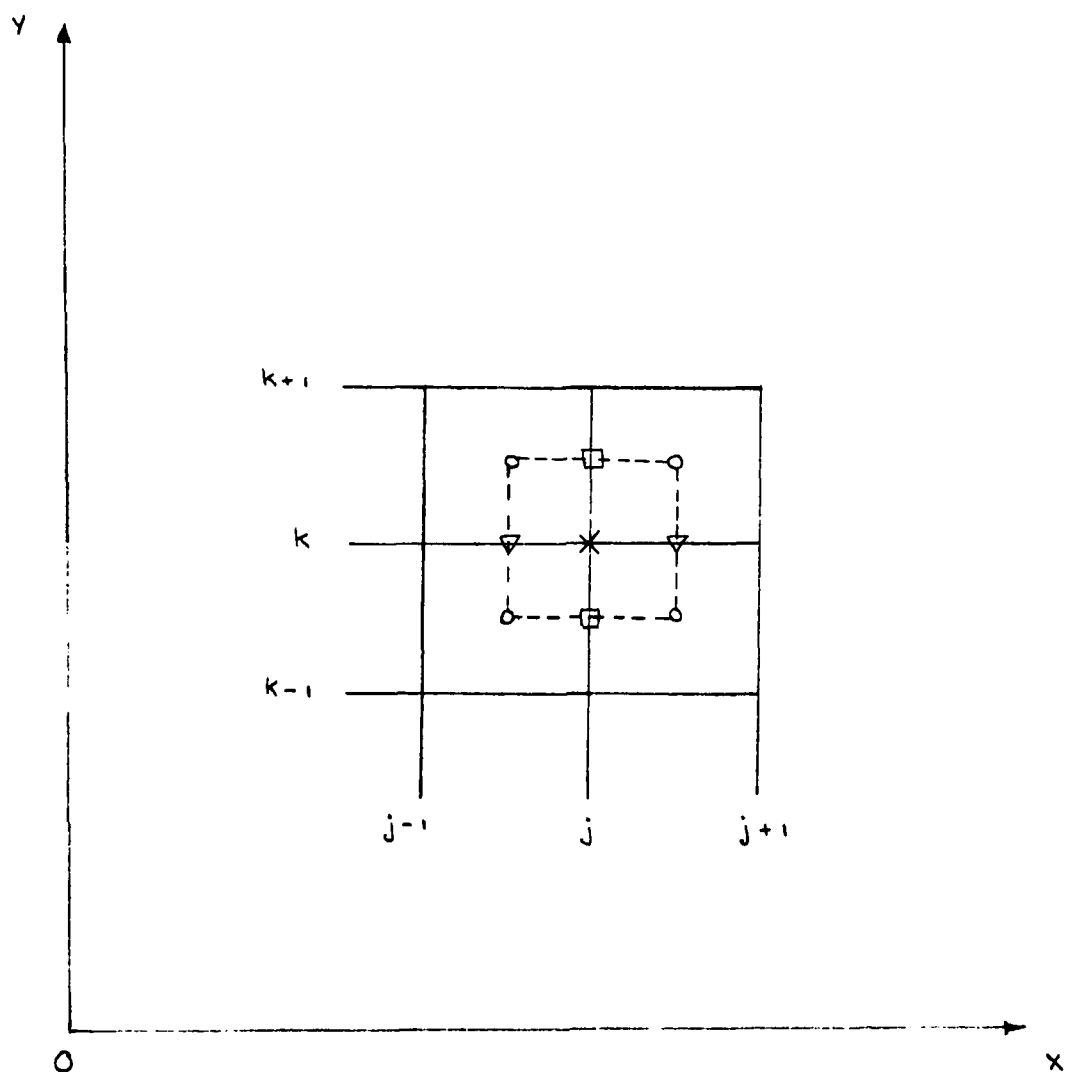
Again  $|\lambda'_n| \leq 1$ , for  $0.5 \leq \epsilon \leq 1$ .

Gray and Pinder employ equation (7.7-7.9) to study the characteristics of the two schemes. An eigenvalue amplitude plot for  $\epsilon = 0.5$  and 1 is developed versus  $\sigma_n \Delta x = (2\pi/L_n)\Delta x = (2\pi/n\Delta x)\Delta x = 2\pi/n$  for  $n \geq 2$  for both (7.12) and (7.14).

Equation (7.8) is employed to provide amplitude ratio plots for both schemes for  $\epsilon = 0.5$  and 1, while, Equation (7.9) is used to develop phase angle plots for  $\epsilon = 0.5$  and 1. Based upon these plots and direct numerical simulation of a step function concentration distribution the spread time derivative scheme is shown superior to the standard time derivative formulation.

#### 8. The Leendertse Formulation

Leendertse [15] considered the space staggered grid illustrated in Figure 7 in applying the finite difference approximations to the following equation sets



- Computational cell
- X Water level ( $\eta$ ) and constituent ( $P$ )
- ▽ x velocity component ( $u$ )
- y velocity component ( $v$ )
- o Water depth ( $h$ )

Figure 7. Leendertse space staggered grid system

$$\frac{\partial (HP)}{\partial t} + \frac{\partial (HuP)}{\partial x} + \frac{\partial (HvP)}{\partial y} - \frac{\partial}{\partial x} \left( HD_x \frac{\partial P}{\partial x} \right) - \frac{\partial \left( HD_y \frac{\partial P}{\partial y} \right)}{\partial y} - HS_A = 0 \quad (8.1)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - fv + g \frac{\partial \eta}{\partial x} + g \frac{u(u^2 + v^2)^{1/2}}{c_H^2} = \frac{1}{\rho H} \tau_x^s \quad (8.2)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + fu + g \frac{\partial \eta}{\partial y} + g \frac{v(u^2 + v^2)^{1/2}}{c_H^2} = \frac{1}{\rho H} \tau_y^s \quad (8.3)$$

$$\frac{\partial \eta}{\partial t} + \frac{\partial (Hu)}{\partial x} + \frac{\partial (Hv)}{\partial y} = 0 \quad (8.4)$$

where

$t \equiv$  time

$x, y \equiv$  Cartesian coordinates

$H \equiv$  water depth

$u, v \equiv$  depth integrated velocities in the  $x$  and  $y$  directions,  
respectively

$f \equiv$  Coriolis parameter

$c \equiv$  Chezy coefficient

$\rho \equiv$  density of water

$\tau_x^s, \tau_y^s \equiv$  surface stresses in the  $x$  and  $y$  directions,  
respectively

$P \equiv$  pollutant concentration

$\eta \equiv$  water surface elevation

$g \equiv$  acceleration of gravity

$D_x, D_y \equiv$  dispersion coefficients in the  $x$  and  $y$  directions,  
respectively

$S_A \equiv$  source strength (concentration/unit/time)

We note in the above equation set that  $P$  is considered an arbitrary pollutant,

The finite difference scheme is ADI with the time step  $\Delta t$  being split in half to advance the solution to  $t + \Delta t$ . In following the finite difference formulations, the reader is referred to Leendertse [15b] for details of notation. In the first sweep from  $t \rightarrow t + \Delta t/2$  the following finite differences are employed in an  $x$  sweep of the grid.

x-sweep  $t \rightarrow t + \Delta t/2$

$j\Delta x \rightarrow x$

$k\Delta y \rightarrow y$

$n\Delta t \rightarrow t$

For continuity we write

$$\begin{aligned} \frac{2}{\Delta t} \left( \eta_{j,k}^{n+1/2} - \eta_{j,k}^n \right) + \left[ \left( h_{j+1/2,k+1/2} + h_{j+1/2,k-1/2} + \eta_{j+1,k}^n \right. \right. \\ \left. \left. + \eta_{j,k}^n \right) u_{j+1/2,k}^{n+1/2} - \left( h_{j-1/2,k+1/2} + h_{j-1/2,k-1/2} + \eta_{j-1,k}^n \right. \right. \\ \left. \left. + \eta_{j,k}^n \right) u_{j-1/2,k}^{n+1/2} \right] \frac{1}{2\Delta x} + \left[ \left( h_{j+1/2,k+1/2} + h_{j-1/2,k+1/2} + \eta_{j,k+1}^n \right. \right. \\ \left. \left. + \eta_{j,k}^n \right) v_{j,k+1/2}^n - \left( h_{j-1/2,k+1/2} + h_{j-1/2,k+1/2} + \eta_{j,k}^n \right. \right. \\ \left. \left. + \eta_{j,k-1}^n \right) v_{j,k-1/2}^n \right] \frac{1}{2\Delta y} = 0 \end{aligned} \quad (8.5)$$



which may be written in general as:

$$-r_{j-1/2} u_{j-1/2,k}^{n+1/2} + \eta_{j,k}^{n+1/2} + r_{j+1/2} u_{j+1/2,k}^{n+1/2} = A_j^n \quad (8.6)$$

For u momentum:

$$\begin{aligned} \frac{1}{\Delta t} \left( u_{j+1/2,k}^{n+1/2} - u_{j+1/2,k}^{n-1/2} \right) - \bar{f} \bar{v} + \frac{\left( u_{j+3/2,k}^{n-1/2} - u_{j-1/2,k}^{n-1/2} \right)}{2\Delta x} u_{j+1/2,k}^{n+1/2} \\ \text{[Centered Difference]} \\ + \left( u_{j+1/2,k+1}^{n-1/2} - u_{j+1/2,k-1}^{n-1/2} \right) \frac{\bar{v}}{2\Delta y} + \left( \eta_{j+1,k}^{n+1/2} - \eta_{j,k}^{n+1/2} + \eta_{j+1,k}^{n-1/2} - \eta_{j,k}^{n-1/2} \right) \frac{\bar{g}}{2\Delta x} \\ \text{[Centered Difference] \quad [Time averaging at } \frac{n+1}{2} \text{]} \\ \text{Derivative centered at} \\ \text{time level } n \\ + \frac{\bar{g} \left( u_{j+1/2,k}^{n+1/2} + u_{j+1/2,k}^{n-1/2} \right) \left[ \left( u_{j+1/2,k}^{n-1/2} \right)^2 + \bar{v}^2 \right]^{1/2}}{(\bar{h}^y + \bar{\eta}^x) (\bar{c}^x)^2} - \frac{1}{p(\bar{h}^y + \bar{\eta}^x)} \tau_x^s = 0 \end{aligned} \quad (8.7)$$

where

$$\begin{aligned} \bar{v} &= \frac{1}{4} \left( v_{j+1,k+1/2}^n + v_{j,k+1/2}^n + v_{j,k-1/2}^n + v_{j+1,k-1/2}^n \right) \\ \bar{h}^y &= \frac{1}{2} \left( h_{j+1/2,k+1/2}^n + h_{j+1/2,k-1/2}^n \right) \\ \bar{\eta}^x &= \frac{1}{2} \left( \eta_{j+1,k}^n + \eta_{j,k}^n \right) \\ \bar{c}^x &= \frac{1}{2} \left( c_{j+1,k}^n + c_{j,k}^n \right) \end{aligned}$$

The above equation may be written in the following form:

$$-r_j \eta_{j,k}^{n+1/2} + r_{j+1/2}^1 u_{j+1/2,k}^{n+1/2} + r_{j+1} \eta_{j+1,k}^{n+1/2} = B_{j+1/2,k}^n \quad (8.8)$$

For the constituent of concern we obtain: (Note i has been dropped, since we are considering only a single constituent.)

$$\begin{aligned}
& \frac{p_{j,k}^{n+1/2} D_{j,k}^{n+1/2} - p_{j,k}^n D_{j,k}^n}{\frac{\Delta t}{2}} - \left[ s_{j-1/2,k}^n u_{j-1/2,k}^{n+1/2} (p_{j-1/2,k}^{n+1/2} + p_{j,k}^{n+1/2}) \right. \\
& - s_{j+1/2,k}^n u_{j+1/2,k}^{n+1/2} (p_{j,k}^{n+1/2} + p_{j+1,k}^{n+1/2}) \left. \right] \frac{1}{4\Delta x} - \left[ s_{j,k-1/2}^n v_{j,k-1/2}^n \right. \\
& \times (p_{j,k-1}^n + p_{j,k}^n) - s_{j,k+1/2}^n v_{j,k+1/2}^n (p_{j,k+1}^n + p_{j,k}^n) \left. \right] \frac{1}{4\Delta y} \\
& + \frac{1}{2(\Delta x)^2} \left[ s_{j-1/2,k}^{n+1/2} x_{j-1/2,k}^{n+1/2} (p_{j,k}^{n+1/2} - p_{j-1,k}^{n+1/2}) - s_{j+1/2,k}^{n+1/2} \right. \\
& \times x_{j+1/2,k}^{n+1/2} (p_{j+1,k}^{n+1/2} - p_{j,k}^{n+1/2}) \left. \right] + \frac{1}{2(\Delta y)^2} \left[ s_{j,k-1/2}^n D_{y,j,k-1/2}^n \right. \\
& \times (p_{j,k}^n - p_{j,k-1}^n) - s_{j,k+1/2}^n D_{y,j,k+1/2}^n (p_{j,k+1}^n - p_{j,k}^n) \left. \right] = 0
\end{aligned} \tag{8.9}$$

where

$$\begin{aligned}
s_{j+1/2,k}^n &= (\eta_{j+1,k}^n + \eta_{j,k}^n + h_{j+1/2,k-1/2} + h_{j+1/2,k+1/2}) \\
s_{j,k+1/2}^n &= (\eta_{j,k+1}^n + \eta_{j,k}^n + h_{j-1/2,k+1/2} + h_{j+1/2,k+1/2})
\end{aligned}$$

This equation is then written in the following general form:

$$a_j p_{j-1,k}^{n+1/2} + b_j p_{j,k}^{n+1/2} + c_j p_{j+1,k}^{n+1/2} = D_j \tag{8.10}$$

Let us now consider the y sweep in which the solution is advanced

from time level  $n+1/2 \rightarrow n$  or  $t + \Delta t/2 \rightarrow t + \Delta t$ . Leendertse expresses the continuity equation as follows:

$$\delta_{+1/2t} \eta + \delta_x [(\bar{h}^y + \bar{\eta}^x)u] + \delta_y [(\bar{h}^x + \bar{\eta}^y)v_t] = 0 \quad j,k,n+1/2 \quad (8.11)$$

where:

$$\begin{aligned} \delta_{+1/2t} \eta &= \frac{\eta_{j,k}^{n+1} - \eta_{j,k}^n}{\frac{\Delta t}{2}} \\ \delta_x [(\bar{h}^y + \bar{\eta}^x)u] &= \delta_x \left[ \left( \frac{h_{j,k+1/2} + h_{j,k-1/2}}{2} + \frac{\eta_{j+1/2,k}^{n+1/2} + \eta_{j-1/2,k}^{n+1/2}}{2} \right) u \right] \\ &= \left[ \left( h_{j+1/2,k+1/2} + h_{j+1/2,k-1/2} + \eta_{j+1/2,k}^{n+1/2} \right. \right. \\ &\quad \left. \left. + \eta_{j,k}^{n+1/2} \right) u_{j+1/2,k}^{n+1/2} - \left( h_{j-1/2,k+1/2} \right. \right. \\ &\quad \left. \left. + h_{j-1/2,k-1/2} + \eta_{j,k}^{n+1/2} + \eta_{j-1,k}^{n+1/2} \right) u_{j-1/2,k}^{n+1/2} \right] / 2\Delta x \\ \delta_y [(\bar{h}^x + \bar{\eta}^y)v_t] &= \delta_y \left[ \left( \frac{h_{j+1/2,k} + h_{j-1/2,k}}{2} + \frac{\eta_{j,k+1/2}^{n+1/2} + \eta_{j,k-1/2}^{n+1/2}}{2} \right) v_t \right] \\ &= \left[ \left( h_{j+1/2,k+1/2} + h_{j-1/2,k+1/2} + \eta_{j,k+1/2}^{n+1/2} \right. \right. \\ &\quad \left. \left. + \eta_{j,k}^{n+1/2} \right) v_{j,k+1/2}^{n+1/2} - \left( h_{j+1/2,k-1/2} \right. \right. \\ &\quad \left. \left. + h_{j-1/2,k-1/2} + \eta_{j,k}^{n+1/2} + \eta_{j,k-1}^{n+1/2} \right) v_{j,k-1/2}^{n+1/2} \right] / 2\Delta y \end{aligned}$$

The  $v$  momentum equation for the  $y$  sweep is given as:

$$\delta_t v + f\bar{u} + \bar{u} \overline{\delta_x v}^x + v_t \overline{\delta_y v}^y + g \overline{\delta_y \eta}^t + g \frac{\bar{v}^t \left[ (\bar{u})^2 + (v_-)^2 \right]^{1/2}}{(\bar{h}^x + \bar{\eta}^y) (\bar{c}^y)^2} - \frac{1}{p(\bar{h}^x + \bar{\eta}^y)} \tau_y^s = 0 \quad \text{at } j, k+1/2, n+1/2 \quad (8.12)$$

where

$$\delta_t v = \frac{v_{j,k+1/2}^{n+1} - v_{j,k+1/2}^{n+1/2}}{\frac{\Delta t}{2}}$$

$$f\bar{u} = f \left( u_{j+1/2,k+1}^{n+1/2} + u_{j+1/2,k}^{n+1/2} + u_{j-1/2,k+1}^{n+1/2} + u_{j-1/2,k}^{n+1/2} \right)$$

$$\overline{\delta_x v}^x = \frac{v_{j+1/2,k+1/2}^n - v_{j-1/2,k+1/2}^n}{\Delta x} = \frac{v_{j+1,k+1/2}^n - v_{j-1,k+1/2}^n}{2\Delta x}$$

$$v_t \overline{\delta_y v}^y = v_{j,k+1/2}^{n+1} \left( \frac{v_{j,k+1}^n - v_{j,k}^n}{\Delta y} \right) = v_{j,k+1/2}^{n+1} \left( \frac{v_{j,k+1/2}^n - v_{j,k-1/2}^n}{2\Delta y} \right)$$

$$\overline{\delta_y \eta}^t = \left( \frac{\eta_{j,k+1}^{n+1} - \eta_{j,k}^{n+1} + \eta_{j,k+1}^n - \eta_{j,k}^n}{2\Delta y} \right)$$

$$\begin{aligned}
\frac{g \bar{v}^t \left[ (\bar{u})^2 + (v_-)^2 \right]^{1/2}}{(\bar{h}^x + \bar{\eta}^y) (\bar{c}^y)^2} &= g \left( \frac{v_{j,k+1/2}^{n+1} + v_{j,k+1/2}^n}{2} \right) \left[ (\bar{u})^2 + (v_{j,k+1/2}^n)^2 \right]^{1/2} \\
&\quad \frac{\left( h_{j+1/2,k+1/2} + h_{j-1/2,k+1/2} + \eta_{j,k+1}^{n+1/2} + \eta_{j,k}^{n+1/2} \right)}{2} \\
&\quad \times \left[ \frac{(c_{j,k+1} + c_{j,k})}{2} \right]^2 \\
\frac{\frac{\tau_y^s}{p}}{(\bar{n}^x + \bar{\eta}^y)} &= \frac{\frac{\tau_y^s}{p}}{\frac{\left( h_{j+1/2,k+1/2} + h_{j-1/2,k+1/2} + \eta_{j,k+1}^{n+1/2} + \eta_{j,k}^{n+1/2} \right)}{2}}
\end{aligned}$$

The constituent equation for the y sweep is expressed as:

$$\begin{aligned}
\delta_{+t/2} [P(\bar{h} + \eta)] + \delta_x [(\bar{h}^y + \bar{\eta}^x) u P^{-x}] + \delta_y [(\bar{h}^x + \bar{\eta}^y) v_t \bar{p}_t^y] \\
- \delta_x [(\bar{h}^y + \bar{\eta}^x) D_x \delta_x P] - \delta_y [(\bar{h}^x + \bar{\eta}^y) D_y \delta_y P_t] = 0 \quad \text{at } j, k, n+1/2
\end{aligned} \tag{8.13}$$

where

$$\delta_{+t/2} [P(\bar{h} + \eta)] = \frac{P_{j,k}^{n+1}(\bar{h} + \eta_{j,k}^{n+1}) - P_{j,k}^{n+1/2}(\bar{h} + \eta_{j,k}^{n+1/2})}{\frac{\Delta t}{2}}$$

with

$$\begin{aligned}
4\bar{h} &= h_{j+1/2,k+1/2} + h_{j+1/2,k-1/2} + h_{j-1/2,k+1/2} \\
&\quad + h_{j-1/2,k-1/2}
\end{aligned}$$

$$\begin{aligned}
\delta_x [(\bar{h}^y + \bar{\eta}^x) u \bar{p}^x] &= \delta_x \left[ \frac{(h_{j,k+1/2} + h_{j,k-1/2} + \eta_{j+1/2,k}^{n+1/2} + \eta_{j-1/2,k}^{n+1/2})}{2} u \right. \\
&\quad \left. \times \frac{(p_{j+1/2,k}^{n+1/2} + p_{j-1/2,k}^{n+1/2})}{2} \right] = \left[ (h_{j+1/2,k+1/2} \right. \\
&\quad + h_{j+1/2,k-1/2} + \eta_{j+1,k}^{n+1/2} + \eta_{j,k}^{n+1/2}) u_{j+1/2,k}^{n+1/2} (p_{j+1,k}^{n+1/2} \\
&\quad + p_{j,k}^{n+1/2}) / 4\Delta x \Big] - \left[ (h_{j-1/2,k+1/2} + h_{j-1/2,k-1/2} \right. \\
&\quad \left. + \eta_{j,k}^{n+1/2} + \eta_{j-1,k}^{n+1/2}) u_{j-1/2,k}^{n+1/2} (p_{j,k}^{n+1/2} + p_{j-1,k}^{n+1/2}) / 4\Delta x \right]
\end{aligned}$$

$$\begin{aligned}
\delta_y [(\bar{h}^x + \bar{\eta}^y) v_t \bar{p}_t^y] &= \delta_y \left[ \frac{(h_{j+1/2,k} + h_{j-1/2,k} + \eta_{j,k+1/2}^{n+1/2} + \eta_{j,k-1/2}^{n+1/2})}{2} v_t \right. \\
&\quad \left. \times \frac{(p_{j,k+1/2}^{n+1} + p_{j,k-1/2}^{n+1})}{2} \right] = \left[ (h_{j+1/2,k+1/2} \right. \\
&\quad + h_{j-1/2,k+1/2} + \eta_{j,k+1}^{n+1/2} + \eta_{j,k}^{n+1/2}) v_{j,k+1/2}^{n+1} (p_{j,k+1}^{n+1} \\
&\quad + p_{j,k}^{n+1}) / 4\Delta y \Big] - \left[ (h_{j+1/2,k-1/2} + h_{j-1/2,k-1/2} \right. \\
&\quad \left. + \eta_{j,k}^{n+1/2} + \eta_{j,k-1}^{n+1/2}) v_{j,k-1/2}^{n+1} (p_{j,k}^{n+1} + p_{j,k-1}^{n+1}) / 4\Delta y \right]
\end{aligned}$$

$$\begin{aligned}
\delta_x \left[ (\bar{h}^y + \bar{\eta}^x) D_x \delta_x P \right] &= \delta_x \left[ \frac{(h_{j,k+1/2} + h_{j,k-1/2} + \eta_{j+1/2,k}^{n+1/2} + \eta_{j-1/2,k}^{n+1/2})}{2} D_x \right. \\
&\quad \times \left. \frac{(p_{j+1/2,k}^{n+1/2} - p_{j-1/2,k}^{n+1/2})}{\Delta x} \right] = \left[ (h_{j+1/2,k+1/2} \right. \\
&\quad + h_{j+1/2,k-1/2} + \eta_{j+1,k}^{n+1/2} + \eta_{j,k}^{n+1/2}) D_{x_{j+1/2,k}}^{n+1/2} (p_{j+1,k}^{n+1/2} \\
&\quad - p_{j,k}^{n+1/2}) / 2\Delta x^2 \Big] - \left[ (h_{j-1/2,k+1/2} + h_{j-1/2,k-1/2} \right. \\
&\quad + \eta_{j,k}^{n+1/2} + \eta_{j-1,k}^{n+1/2}) D_{x_{j-1/2,k}}^{n+1/2} (p_{j,k}^{n+1/2} - p_{j-1,k}^{n+1/2}) / 2\Delta x^2 \Big] \\
\delta_y \left[ (\bar{h}^x + \bar{\eta}^y) D_y \delta_y P \right] &= \delta_y \left[ \frac{(h_{j+1/2,k} + h_{j-1/2,k} + \eta_{j,k+1/2}^{n+1/2} + \eta_{j,k-1/2}^{n+1/2})}{2} D_{y_t} \right. \\
&\quad \times \left. \frac{(p_{j,k+1/2}^{n+1} - p_{j,k-1/2}^{n+1})}{\Delta y} \right] = \left[ (h_{j+1/2,k+1/2} \right. \\
&\quad + h_{j-1/2,k+1/2} + \eta_{j,k+1}^{n+1/2} + \eta_{j,k}^{n+1/2}) D_{y_{j,k+1/2}}^{n+1} \\
&\quad \times (p_{j,k+1}^{n+1} - p_{j,k}^{n+1}) / 2\Delta y^2 \Big] - \left[ (h_{j+1/2,k-1/2} \right. \\
&\quad + h_{j-1/2,k-1/2} + \eta_{j,k}^{n+1/2} + \eta_{j,k-1}^{n+1/2}) D_{y_{j,k-1/2}}^{n+1} \\
&\quad \times (p_{j,k}^{n+1} - p_{j,k-1}^{n+1}) / 2\Delta y^2 \Big]
\end{aligned}$$

Note that the above equation may be written as

$$a_{k-1} p_{j,k-1}^{n+1} + b_k p_{j,k}^{n+1} + c_{k+1} p_{j,k+1}^{n+1} = D_k$$

In this approach the constituent equation is solved directly within the hydrodynamic computation sweeps although there is no coupling.

In the application to Jamaica Bay, salient simulation characteristics are as follows:

a.  $\Delta s = \Delta x = \Delta y = 500 \text{ ft (15.24 m)}$

$$\Delta t = 120 \text{ sec}$$

b. The explicit time step,  $\Delta t_e$ , is given as follows.

$$\Delta t_e = \frac{\Delta s}{\sqrt{gD_{\max}}} = \frac{500}{40} = 12.5 \text{ sec}$$

c. The gravity wave Courant number  $Cr_w$  is given by

$$Cr_w = \frac{\Delta t}{\Delta t_e} \approx 10$$

d. The particle Courant number  $Cr_p$  is given by

$$Cr_p = \frac{u \Delta t}{\Delta s} = \frac{(0.5 \text{ ft/sec}^*)(120 \text{ sec})}{500 \text{ ft}^{**}} = 0.0120$$

e. The dispersion coefficient formulation is given by

$$D_x = 14.3 \sqrt{2g} u H c^{-1} + D_w, \text{ where } D_w \in (25, 45) \text{ ft}^2/\text{sec}^{\dagger}$$

where

$D_x \equiv$  dispersion coefficient

$g \equiv$  gravity

---

\* 0.1524 m/sec.  
 \*\* 152.4 m.  
 † 232,4.18 m<sup>2</sup>/sec.



$c \equiv$  Chezy coefficient

$H \equiv$  local water depth

$D_w \equiv$  background dispersion coefficient

f. The Chezy coefficient is given by

$$c = \frac{1.49}{nR^{1/6}} \approx \frac{1.49}{(0.01)(11)} \approx 100$$

where

$c \equiv$  Chezy coefficient

$R \equiv$  hydraulic radius

$n \equiv$  Manning's roughness

g. The dispersion coefficient used becomes

$$D_x = \frac{(112)(0.5)(25)}{100} + 25 = 37.5 \text{ ft}^2/\text{sec} [3.484 \text{ m}^2/\text{sec}]$$

with

$$\frac{D_x \Delta t}{\Delta s^2} = \frac{(37.5)(120)}{250,000} = 0.018$$

and a cell Peclet number,  $Pe = \frac{u \Delta x}{D_x} = \frac{(0.5)(500)}{37.5} = 6.7$

## 9. Additional Methods and Considerations

Bram van Leer [16, 17] has developed several upstream centered higher order convective schemes. His work is highly theoretical within the domain of numerical analysis but seems to indicate a general approach to constructing extremely accurate finite difference schemes.

Forester [18] has presented a non-linear filtering technique for higher order even (greater than two) finite difference schemes which preserves the peak of an external type distribution unlike flux corrected transport filtering. The application of the filter to points near the boundary was not reported and the determination of the coefficients must be made through direct numerical experimentation for each problem individually.

Narayan and Shankar [19] have employed a multi-operational scheme similar to the Leendertse scheme previously outlined in an application to Galveston Bay. Oster et al. [20] employed Leendertse's scheme [15] with upwind differencing in a two-dimensional computation. Hinstrup et al. [21] at Danish Hydraulic Institute have developed a two-dimensional explicit scheme employing 12 point Everett interpolation. The treatment of boundary cells appears to result in some mass falsification.

Runchal [22], Siemieniuch and Gladwell [23], and Lillington and Shepherd [24] demonstrate the oscillatory nature of central difference approximation to the steady state equation in convection dominated problems for cell Peclet numbers greater than 2. Jensen and Finlayson [25] note this oscillatory behavior may be observed in transient simulations of sharp fronts as well for improper time and space scales.

Molenkamp [26] has provided a review of several finite difference approximations and compared them for a rotation of a circular distribution. This test problem provides for a non-uniform velocity field

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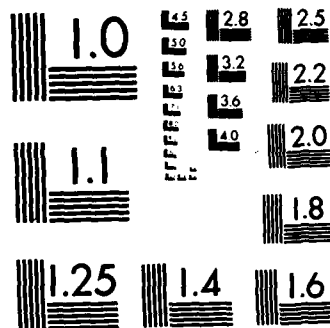
THE DEVELOPMENT OF A NUMERICAL SOLUTION TO THE  
TRANSPORT EQUATION REPORT 1 METHODOLOGY(U) COASTAL  
ENGINEERING RESEARCH CENTER VICKSBURG MS R A SCHMALZ  
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MICROCOPY RESOLUTION TEST CHART  
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within two dimensions and will be employed as a test case for the to be developed salinity algorithms.

The cell Peclet number as mentioned above plays a major role in characterizing the relationship between the grid resolution and the numerical scheme. It is defined as

$$Pe_x = \frac{\Delta x u}{K_x} \quad Pe_y = \frac{\Delta y v}{K_y} \quad (9.1)$$

where

$\Delta x \equiv$  grid spacing

$u \equiv$  maximum magnitude of the velocity in the  $x$  direction

$v \equiv$  maximum magnitude of the velocity in the  $y$  direction

$K_x \equiv$  dispersion coefficient in the  $x$  direction

$K_y \equiv$  dispersion coefficient in the  $y$  direction

The Peclet number limit of two is required to prevent oscillations in the solution in the vicinity of a sharp concentration front for central space differencing. For typical velocities and dispersion coefficients,  $\Delta x$  and  $\Delta y$  would be in the scale of hundreds of feet. This space scale is too severe to be applied over the entire area of Mississippi Sound. The Peclet number limit, however, is only significant for sharp fronts and although there may be significant horizontal gradients in salinity, these gradients are not as severe as a shock or discontinuity in the distribution. If first order upstream differences are applied no oscillations will develop, but accuracy limitations (such as those developed by Leonard [27]) usually require a dense grid. In practical

computations, one normally decides on a space scale of significance,  $S$ , and selects the grid spacings,  $\epsilon$ , such that  $\epsilon \leq S/10$ . Higher order schemes may allow this limitation to be relaxed. However, these higher order methods normally involve more complicated algorithms and increased computational cost and model development time.

In conclusion, it should be noted that there is no one best computational finite difference scheme for the transport equation. However, the necessity to perform computations over a two-dimensional grid with irregular boundaries, suggests that a simpler lower order method be selected which is not too inaccurate.

#### PART IV: NUMERICAL METHOD SELECTION AND DEVELOPMENT

The method of solution for the transport equation must be compatible with the hydrodynamic scheme employed in WIFM. Since the convective terms must be treated in the hydrodynamics for tidal circulation, the following explicit type time step limitation must be obeyed

$$u\Delta t \leq \min \left( \frac{\Delta x \Delta y}{\sqrt{\Delta x^2 + \Delta y^2}} \right) = \min \left[ \left( \frac{\text{Area}}{\text{Diagonal}} \right) \right] \quad (3.1)$$

where

$u \equiv$  maximum particle velocity magnitude

$\Delta x \equiv$  spatial increment in  $x$  direction (variable)

$\Delta y \equiv$  spatial increment in  $y$  direction (variable)

It is desirable to leave open the option of coupling the salinity transport through an equation of state to the density involved in the pressure gradient terms within the hydrodynamics. If this is to be accomplished the method of solution of the transport equation must also satisfy the above equation. This allows both explicit and implicit methods for solution to the transport equation to be considered. Explicit methods must obey (3.1), whereas for implicit methods the only time step limit is one of accuracy.

If density coupling is not necessary and explicit methods are employed then it may be possible to employ a time step in the transport solution,  $\Delta t^T = n \Delta t^H$ , where  $n$  is an integer and  $\Delta t^H$  is the time step in the hydrodynamic solution. In this case the following limit

must be obeyed for an explicit method

$$\bar{u}\Delta t^T \leq \min \left( \frac{\Delta x \Delta y}{\sqrt{\Delta x^2 + \Delta y^2}} \right) \quad (3.2)$$

where  $\bar{u}$  represents the maximum magnitude of the particle velocity averaged over  $n\Delta t^H$ . The explicit time step transport limit will be less than an implicit time step transport limit. Thus an implicit method may accommodate larger time steps than an explicit method. Leendertse [15] notes the problem of conservation in averaging velocity fields. However, in order to develop long term transport patterns, it may be desirable to employ much larger time steps in the transport equation solution than in the hydrodynamics. For this reason and to maintain consistency of approach with the hydrodynamics a multi-operational implicit scheme will be developed for the transport equation.

As has been previously presented, the work of Stone and Brian [13] and Gray and Pinder [14] illustrate the improved computational characteristics of the spread time derivative method over the standard forward time centered space method in one-dimensional problems. Siemon [28] has investigated the extension of the method to semi two dimensional problems (advection in one coordinate direction, diffusion in both coordinate directions) and reported favorable results. To the author's knowledge, the extension to completely two dimensional problems has not been reported. It is proposed that this extension be investigated in this project. By employing appropriate coefficients in the numerical formulation, the method could be degenerated to Leendertse's approach.



In this manner, two computational schemes may be coded in one operation. The format of the spread time derivative scheme is such that it may not be expressed in a form suitable to flux corrected transport. As a result, oscillations in the solution may be smoothed using filtering techniques. The necessity of filtering cannot be determined until numerical experiments are conducted.

As an alternative, Leendertse's approach will be implemented with flux correction. The higher order scheme will correspond to the standard Leendertse formulation. The lower order scheme will employ upwind differencing of the advective terms. Thus, two schemes must effectively be programmed (a higher and lower order scheme) for flux correction.

The two alternative schemes spread time derivative and Leendertse flux corrected will be compared through numerical experimentation to determine the most appropriate technique for application in Mississippi Sound.

The flux correction method is such that any higher order method may be employed. Leendertse's method is  $O(\Delta t^2, \Delta x^2, \Delta y^2)$  and is amenable to adaptation to variable grid spacing using the exponential stretch transformation in WIFM. In the future, it may be desirable to consider higher order compact differencing schemes such as the Kreiss scheme as reported by Roache [29]. The flux correction method will accommodate further research in the development and implementation of higher order schemes.

The general strategy and development of the numerical approximations to the transport equation for application to Mississippi Sound is

shown in Figure 8. This approach provides for development of an optimal second order method.

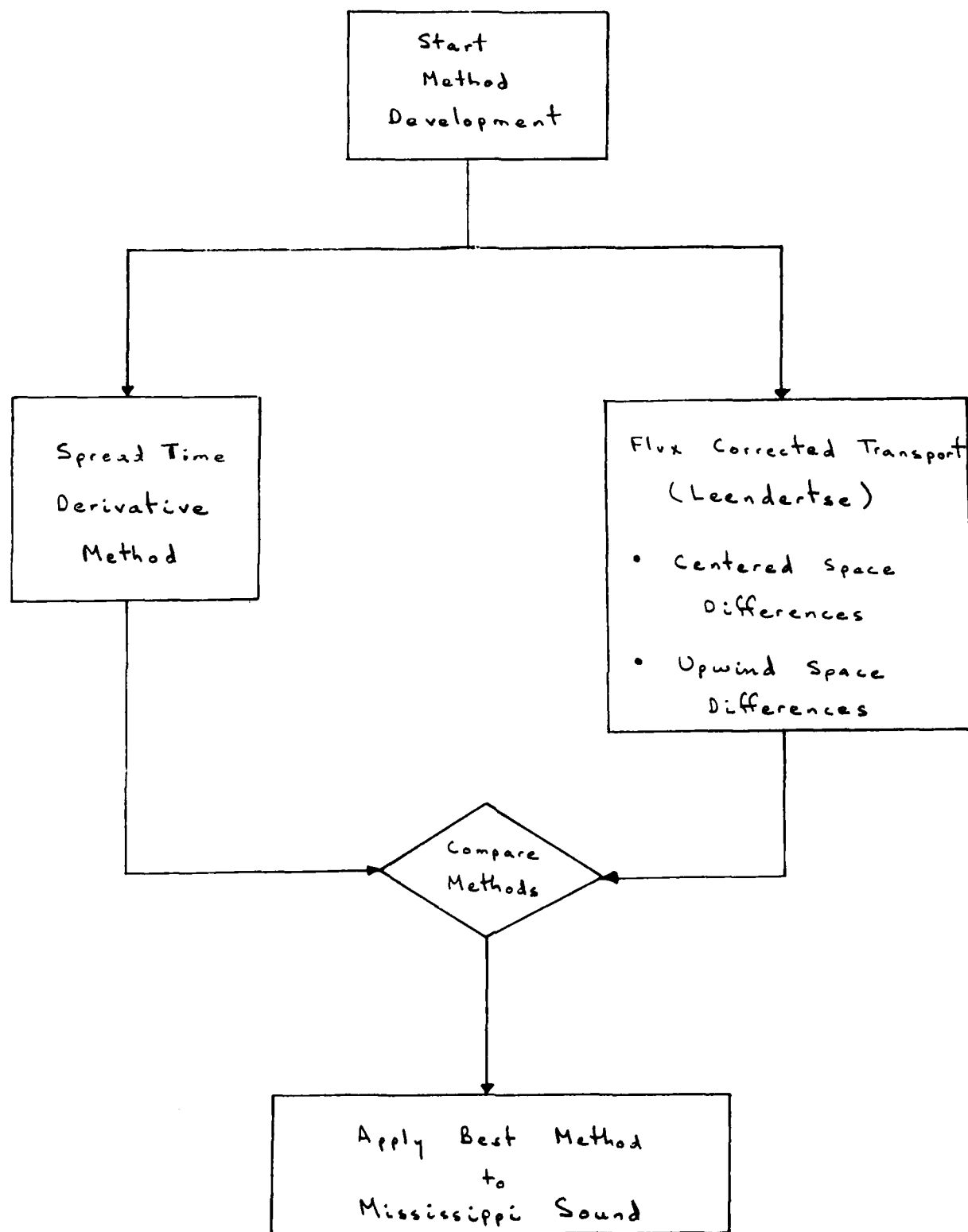


Figure 8. Development of a numerical method for the transport equation

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